ANNUAL REPORT

2005

RESEARCH INSTITUTE FOR SOLID STATE
PHYSICS AND OPTICS
Hungarian Academy of Sciences, Budapest, Hungary

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RESEARCH INSTITUTE FOR SOLID STATE
PHYSICS AND OPTICS
Hungarian Academy of Sciences, Budapest, Hungary

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Hungarian Academy of Sciences

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ANNUAL REPORT 2005

Edited by **L. Csillag, G. Konczos, B. Selmeci, I. Tüttő**

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Dear Reader,

It is my pleasure to hand over the 12th, 2005 edition of the Annual Report of the Research Institute for Solid State Physics and Optics.

Our institute was founded by the *Hungarian Academy of Sciences* in 1981 as part of the *Central Research Institute for Physics*. In 1992 we became an independent institute under the name of *Research Institute for Solid State Physics*. The present profile of the institute took shape in 1998 when the *Crystal Physics Laboratory* of the Hungarian Academy of Sciences joined us, and our name changed to *Research Institute for Solid State Physics and Optics*.

The primary mission of the institute is conducting basic research in the fields of theoretical and experimental solid state physics and materials science including metal physics, crystal physics and liquid crystal research, theoretical and experimental optics including laser physics, quantum optics and the interaction of light with matter. Our experimental research activity is connected to unique methodologies like X-ray diffraction, NMR-, Mössbauer-, and optical spectroscopy and neutron scattering experiments at the *Budapest Neutron Centre*. Some of our research activities are closely related to applications, e.g., in the fields of optical thin films, laser applications, crystal growing technologies and metallurgy.

About 60 % of our funding is provided by the Hungarian Academy of Sciences; the rest originates from a variety of funding agencies in the form of competitive projects. Basic research is financed mostly by the *Hungarian Research Fund* (OTKA, 46 projects). During the past years our participation in large-scale national applied research and development programs has increased considerably (11 NKFP projects in 2005). These projects are typically implemented in cooperation with universities and industrial partners with the aim of improving the competitiveness of the Hungarian economy. This year the institute was awarded 167 million HUF in the framework of the *Economic Competitiveness Operational Programme* (GVOP). A consortium of four institutes of the Hungarian Academy of Sciences lead by our institute gained support from the *National Office for Research and Technology* in the *Large International Projects* programme (NAP, 400 million HUF).

Our staff consists of 185 employees with 129 scientists among them. Thanks to a long tradition of our graduate and postgraduate training programmes, more and more young researchers are joining us. We are involved in several international projects in collaboration with a great number of research institutions and universities. More than half of our publications (about 55 %) feature co-authors from foreign countries indicating an essential role of these partnerships. Various EU, ESF, COST, NATO and other international projects

play an important role in our research activity. The share of these international resources in our budget is about 9 % (see Key figures).

This year we have published 198 papers in high quality peer-reviewed international journals as well as 40 papers in conference proceedings or books. These numbers are similar to those in previous years. We are proud that Norbert Kroó, our former director, has received the award *De Scientia et Humanitate Optime Meritus* from the Academy of Sciences of the Czech Republic. Two of our scientists, László Gránásy and Ferenc Iglói won the *Physics Award* of the Hungarian Academy of Sciences, and Zoltán Donkó became *Doctor of the Hungarian Academy of Sciences* (DSc) this year. Two of our researchers won Bolyai Grants in 2005. It is a tradition in our institute to present awards for outstanding publication activity. In 2005 the publication prize was won by Lajos K. Varga for his work in the field of soft magnetic nanocrystalline alloys.

In addition to the new scientific results, several improvements have been achieved in our infrastructure. A new laboratory to study ultrashort laser pulses has been installed, and there have been significant reconstruction measures in our main building.

I hope that this booklet gives useful information to the reader. The key figures will help you to get a general overview of our institute. In addition to the description of the research activities, the Annual Report contains the e-mail addresses of our scientists as well for an easier contact. For further information please visit our WEB page at http://www.szfki.hu.

Budapest, 30 November, 2005

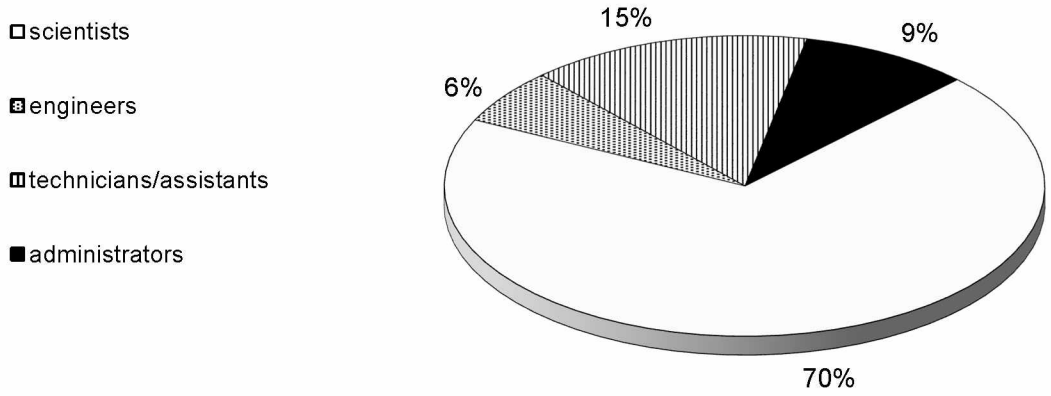
János Kollár

Director

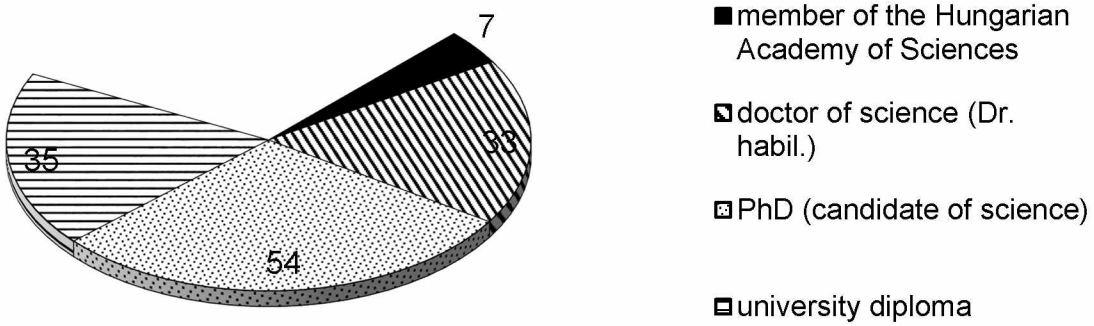
Key figures

Permanent staff of the Institute: 185 employees. Its distribution:

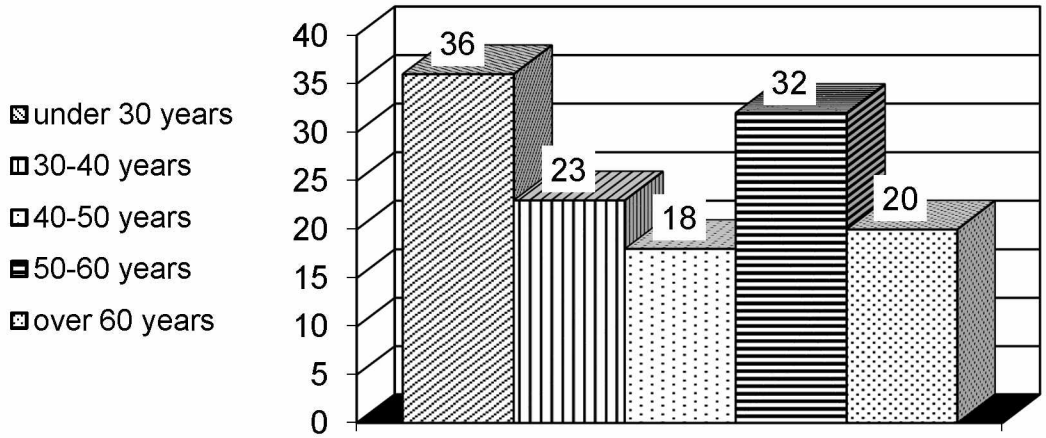
a) by professions:



b) by scientific titles/degrees:

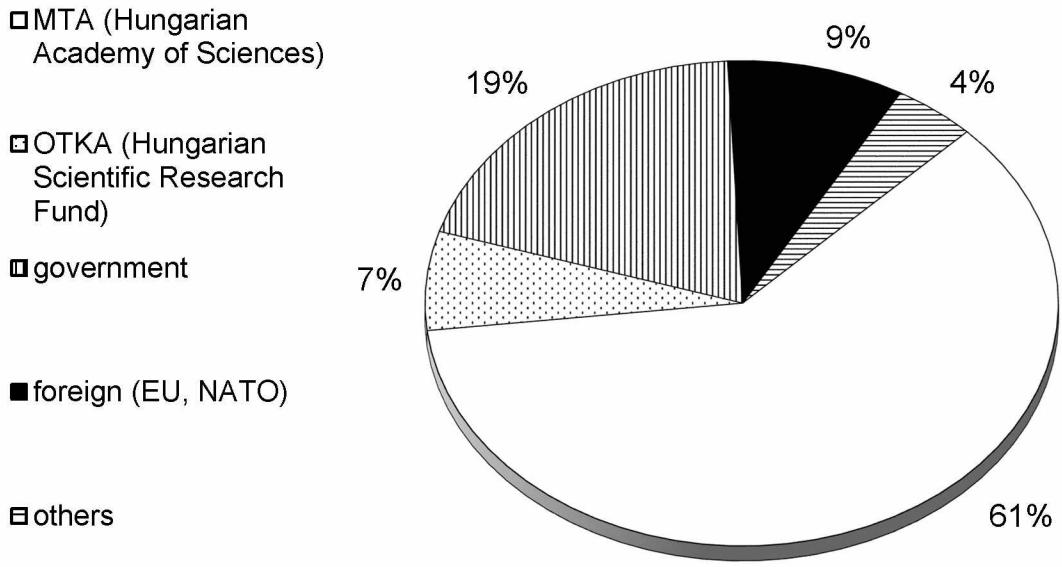


c) by ages:

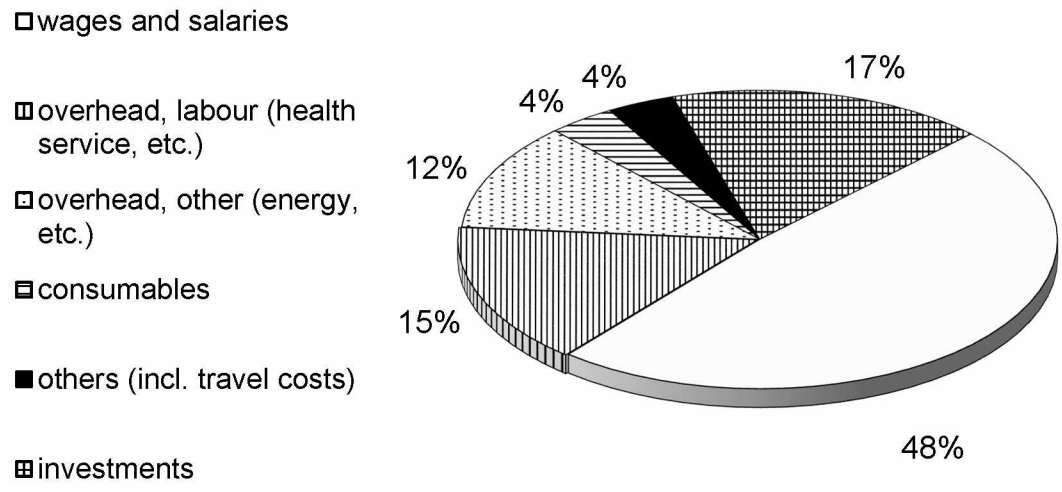


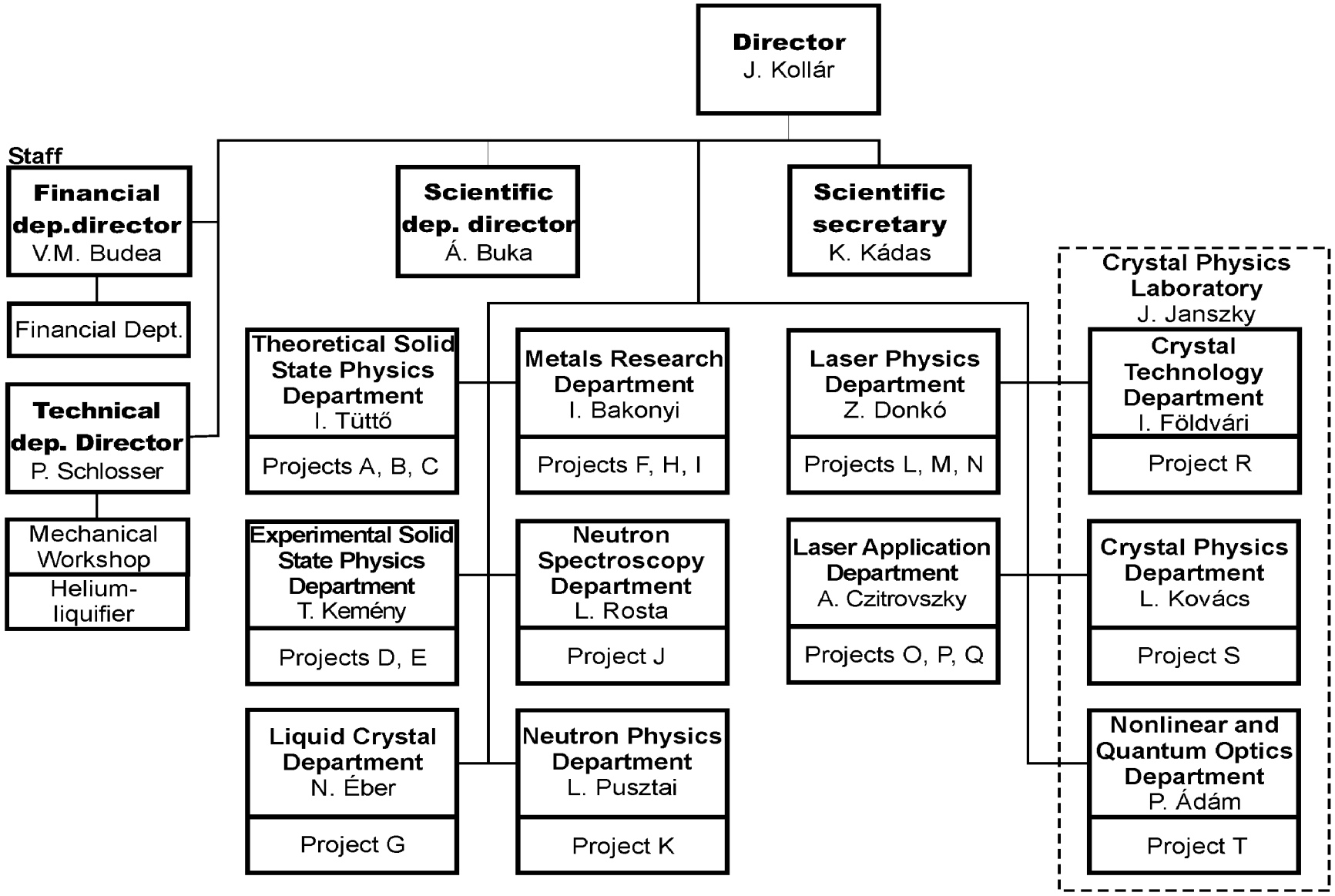
Financial management

a) Sources of operation costs:



b) Distribution of expenditures:





Structure of the Research Institute for Solid State Physics and Optics

A. STRONGLY CORRELATED SYSTEMS

J. Sólyom, K. Buchta[#], G. Fáth, Ö. Legeza, K. Penc, E. Szirmai[#], K. Vladár, F. Woynarovich, A. Zawadowski[+]

Low-dimensional fermionic and spin models. — We have continued the application of the density-matrix renormalization-group (DMRG) method to fermionic and spin systems. The ground-state phase diagram of the bilinear-biquadratic spin-1 chain has been studied near the ferromagnetic instability point, where the existence of a gapped or gapless nondimerized quantum nematic phase has been suggested. Our results are consistent with the view that the order parameter characterizing the dimer phase vanishes only at the point where the system becomes ferromagnetic, although the existence of a gapped or gapless nondimerized phase in a very narrow parameter range between the ferromagnetic and the dimerized regimes cannot be ruled out.

We have proposed a new approach to locate quantum phase transitions in low-dimensional lattice models using DMRG. It is demonstrated on the example of fermionic and spin models that the von Neumann entropy of the ensemble of two neighboring sites in a long chain is a better indicator of quantum phase transitions than calculating gaps or order parameters. This has been used to determine the nature of the neutral-ionic transition in organic mixed-stack compounds. A unified model has been derived which, in limiting cases, is equivalent to the models proposed earlier, the donor-acceptor model and the ionic Hubbard model. The new procedure allowed us to get a unified phase diagram.

We have presented an analysis of a system of weakly coupled Hubbard chains based on combining an exact study of spectral functions of the uncoupled chain system with a renormalization group method for the coupled chains. For low values of the onsite repulsion and doping, the leading instability is towards a superconducting state. The process included excited states above a small correlation pseudogap. Similar features appear in extended Hubbard models in the vicinity of commensurate fillings. Our theoretical predictions are consistent with the phase diagram observed in the $(TMTTF)_2X$ and $(TMTSF)_2X$ series of organic compounds.

Low-dimensional and frustrated magnetic systems. — Using classical Monte Carlo simulations, we have determined the finite-temperature phase diagram and thermodynamic properties of the antiferromagnetic Heisenberg model on a pyrochlore lattice under external magnetic field. The model includes bilinear and biquadratic interactions; the latter effectively describes the coupling to lattice distortions. The magnetization process shows a half-magnetization plateau at low temperatures, accompanied by strong suppression of the magnetic susceptibility. The results are compared with recent experimental results in $CdCr_2O_4$ and $HgCr_2O_4$ chromium spinel oxides.

Other problems. — We have mapped the problem of a resonant level impurity interacting with the conduction band by a finite-range interaction onto that of a 1d Coulomb gas. Scaling was performed and the fixed-point Hamiltonian was determined. We could handle arbitrary number of electron scattering channels. Upon examining some simple models we have found different types of low temperature behavior.

A general theory of cultural evolution has been formulated using a cognitive dimension-reduction scheme. Rational but cognitively limited agents iteratively invent and redefine

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[#] PhD student

[+] Permanent position: Budapest University of Technology and Economics

abstract concepts in order to best represent their natural and social environment. These concepts are used for decision making and determine the agents' overall behavior. The collection of concepts an agent uses constitutes his/her cultural profile. As the importance of social interactions increases and/or agents become more intelligent we find a series of dynamical phase transitions by which the coherence of concepts advances in the society. Our model explains the so-called "cultural explosion" in human evolution 50,000 years ago as a spontaneous ordering phenomenon of the individual mental representations.

We have presented a model in which abstract concepts of a language acquire meaning as the result of competition between heterogeneous interacting agents in a community. We argue that bounded rationality requires individuals to use a reduced number of abstract concepts to represent the rich reality of the world. The meanings of these concepts emerge as a trade-off between two objectives: (i) agents want to use concepts that are best adopted to their idiosyncratic preferences and characteristic distribution of choice alternatives, (ii) agents seek to share concepts to benefit from communication. Agents play a non-cooperative game, whose Nash equilibrium determines the collective meanings of concepts in the population, constituting together the community's language. Analysis of the possible Nash equilibria and the evolutionary game dynamics shed light on interesting theoretical questions such as the origins of meaning, the coherence of language, the language-culture relationship, and Whorf's hypothesis on linguistic relativism.

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Grants

OTKA T043330	Theoretical study of strongly correlated low-dimensional systems (J. Sólyom, 2003-2006)
OTKA F046356	Development and application of the momentum-space density-matrix renormalization-group method for fermionic systems (Ö. Legeza, 2004-2007)
OTKA T047003	Statistical physics of evolutionary games (Participant: G. Fáth, 2004-2007)
OTKA T049607	Exotic phases and excitation in frustrated electron systems with charge, spin and orbital degrees of freedom (K. Penc, 2005-2007)
NKFP 2/051/2004	Language Miner (Participant: G. Fáth, 2005-2007)

Publications

Articles

A.1. Carmelo* JMP, Guinea* F, Penc K, Sacramento* PD; Superconductivity driven by chain coupling and electronic correlations; *Europhys Lett*; **68**, 839-845, 2004

A.2. Szirmai E, Sólyom J; Mott transition in the one-dimensional SU(n) Hubbard model; *Phys Rev B*; **71**, 205108/1-7, 2005

A.3. Buchta K, Fáth G, Legeza Ö, Sólyom J; Probable absence of a quadrupolar spin-nematic phase in the bilinear-biquadratic spin-1 model; *Phys Rev B*; **72,** 054433/1-6, 2005

A.4. Legeza Ö, Sólyom J; Entropic signature of quantum phase transitions in low-dimensional models; *cond-mat*/0511181, 2005

A.5. Legeza Ö, Buchta K, Sólyom J; Unified phase diagram of models exhibiting neutral-ionic transition; *cond-mat*/0511182, 2005

A.6. Motome* Y, Tsunetsugu* H, Hikihara* T, Shannon* N, Penc K; Interplay among spin, orbital and lattice degrees of freedom in t_{2g} electron systems with edge-sharing network of octahedra; *Prog Theor Phys Suppl*; **159**, 314-318, 2005

A.7. Carmelo* JMP, Penc K, Bozi* D; Finite-energy spectral-weight distributions of a 1D correlated metal; *Nucl Phys B*; **725**, 421-466, 2005

A.8. Carmelo* JMP, Guinea* F, Penc K, Sacramento* PD; Application of the pseudofermion dynamical theory to the properties of quasi-1D compounds; *Physica B*; **359**, 1427-1429, 2005

A.9. Fáth G, Sarvary* M; A renormalization group theory of cultural evolution; *Physica A*; **348**, 611-629, 2005

A.10. Motome* Y, Penc K, Shannon* N; Monte-Carlo study of half-magnetization plateau and magnetic phase diagram in pyrochlore antiferromagnetic Heisenberg model; *J Magn Magn Mat*; accepted for publication

Conference proceeding

A.11 Fáth G, Sarvary* M; Towards an economic theory of meaning and language; In: *Proceedings of ECCS'05, Nov 14-18 2005, Paris*; accepted for publication

Book chapter

A.12 Fáth G, Sarvary* M; Cultural evolution in a population of heterogeneous agents; In: *Economics and Heterogeneous Interacting agents, Lecture notes in economics and mathematical systems*, Eds.: A. Namatame, T. Kaizouji, Y. Aruka; accepted for publication

B. COMPLEX SYSTEMS

F. Iglói, N. Menyhárd, A. Sütő, P. Szépfalusy

The principal interest of this group is the theoretical investigation of different aspects of equilibrium and non-equilibrium statistical physics and quantum systems.

Phase transitions and critical behaviour. — We have studied the one-dimensional partially asymmetric exclusion process with random hopping rates, in which a fraction of particles (or sites) have a preferential jumping direction against the global drift. In this case the accumulated distance traveled by the particles, x, scales with the time, t, as $x \sim t^{1/z}$, with a dynamical exponent $z > 0$. Using extreme value statistics and an asymptotically exact strong disorder renormalization group method we exactly calculate, z_{pr}, for particlewise (pt) disorder, which is argued to be related as, $z_{st}=z_{pr}/2$, for sitewise (st) disorder. In the symmetric model with zero mean drift the particle diffusion is ultra-slow, logarithmic in time.

We have written a review article about the use of the strong disorder renormalization group (RG) method for random systems. This method can be used for a large variety of quantum and classical systems in which the quenched disorder plays a dominant role over quantum, thermal, or stochastic fluctuations: these systems display strong spatial heterogeneities, and many averaged observables are actually governed by rare regions. We have reported these new developments by starting with an introduction of the main ingredients of the strong disorder RG method. We have described the basic properties of infinite disorder fixed points, which are realized at critical points, and of strong disorder fixed points, which control the singular behaviors in the Griffiths-phases. We have also reviewed in detail applications of the RG method to various disordered models, either (i) quantum models, such as random spin chains, ladders and higher dimensional spin systems, or (ii) classical models, such as diffusion in a random potential, equilibrium at low temperature and coarsening dynamics of classical random spin chains, trap models, delocalization transition of a random polymer from an interface, driven lattice gases and reaction diffusion models in the presence of quenched disorder. For several one-dimensional systems, the RG rules yield very detailed analytical results, whereas for other, mainly higher dimensional problems, the RG rules have to be implemented numerically. If available, the strong disorder RG results are compared with another, exact or numerical calculations.

An investigation of the effect of quenched disorder in one-dimensional non-equilibrium Ising-like spin systems also with inherent spin asymmetry has been carried out via computer simulations. In the strong disorder limit characteristic changes appear in the time-dependent as well as in the static critical behavior.

Quantum systems. — Investigations of quantum gases have been continued in this year. In case of the spinor Bose gas we have shown that the magnetic phase transition (prior to the BEC) is accompanied by a creation of two phases with different densities. At the critical point the soft mode has been found and studied. In Fermi gases consisting of atoms with spins higher than 1/2 further properties of clustering have been explored.

We extended the effective meson model used previously to include the kaon and pointed out the change of the order of the chiral phase transition when the masses of the pion and the kaon are varied. The temperature dependences of the strange and the non-strange condensates have been followed.

In two papers the question of the equivalence of Bose-Einstein condensation and the spontaneous breakdown of the gauge symmetry has been answered positively. In the first

paper simplified mean-field and perturbed mean-field interactions were considered. The second paper contains the proof for the case of general interactions.

Other researches. — The charge flipping method of phase retrieval in crystallography, introduced last year, has been further developed. During iteration, in Fourier space a 90 degrees phase shift is applied to the structure factors of weak reflections. This drastically improves convergence, in some cases makes earlier unresolved structures solvable.

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András Sütő	suto@szfki.hu
Péter Szépfalusy	psz@galahad.elte.hu

Grants and international cooperations

OTKA T048721 Statistical physics of disordered systems (F. Iglói, 2005-2008)

OTKA T046129 Dynamics of phase transitions and symmetry breaking phases (P. Szépfalusy, 2004-2007)

OTKA T042914 Mathematical study of interacting Fermi and Bose systems (A. Sütő, 2003-2005)

DAAD-MÖB 4/2004 Statistical physics of nonequilibrium and disordered systems (F. Iglói, 2004-2005)

TéT F-17/03 (Hungarian-French) Statistical physics of disordered systems (F. Iglói, 2004-2005)

Publications

Articles

B.1. Juhász* R, Santen* L, Iglói F; Partially asymmetric exclusion models with quenched disorder; *Phys Rev Lett;* **94**, 010601/1-4, 2005

B.2. Pleimling* M, and Iglói F; Nonequilibrium critical dynamics in inhomogeneous systems; *Phys Rev B*; **71**, 094424/1-12, 2005

B.3. Mercaldo* MT, d'Auriac* AJ-Ch, Iglói F; Disorder driven phase transitions of the large q-state Potts model in *3d*; *Europhys Lett;* **70**, 733-739, 2005

B.4. Iglói F, Monthus* C; Strong disorder RG approach of random systems; *Physics Reports;* **412**, 277-431, 2005

B.5. Mélin* R, Douçot* B, Iglói F; Strong disorder renormalization group on fractal lattices: Heisenberg models and magnetoresistive effects in tight binding models; *Phys Rev B*; **72,** 024205/1-17, 2005

B.6. Bagaméry* FÁ, Turban* L, Iglói F; Two-dimensional Ising model with self-dual biaxially correlated disorder; *Phys Rev B*; **72**, 094202/1-9, 2005

B.7. Lajkó* P, Carlon* E, Rieger* H, Iglói F; Disorder Induced Phases in the $S=1$ Antiferromagnetic Heisenberg Chain; *Phys Rev B*; **72**, 094205/1-7, 2005

B.8. Juhász* R, Santen* L, Iglói F; The partially asymmetric zero range process with quenched disorder; *Phys Rev E*; **72**, 046129/1-12, 2005

B.9. Kis-Szabó* K, Szépfalusy P, Szirmai* G; Static properties and spin dynamics of the ferromagnetic spin-1 Bose gas in a magnetic field; *Phys Rev A*; **72**, 023617/1-8, 2005

B.10. Szirmai* G, Kis-Szabó* K, Szépfalusy P; Phase separation of ferromagnetic spin-1 Bose gases in non-zero magnetic field; *Eur Phys J D;* **36**, 281-287, 2005

B.11. Herpay* T, Patkós* A, Szép* Zs, Szépfalusy P; Mapping the boundary of the first order finite temperature restoration of chiral symmetry in the m_{pi} - m_K -plane with a linear sigma model; *Phys Rev D*; **71**, 125017/1-15, 2005

B.12. Sütő A; Bose-Einstein condensation and symmetry breaking; *Phys Rev A*; **71**, 023602/1-8, 2005

B.13. Sütő A; Equivalence of Bose-Einstein condensation and symmetry breaking; *Phys Rev Lett;* **94**, 080402/1-4, 2005

See also E.6., E.14.

C. ELECTRONIC STATES IN SOLIDS

J. Kollár, P. Fazekas, K. Kádas, B. Lazarovits, I. Tüttő, B. Újfalussy, A. Virosztek[+], L. Vitos, V Zólyomi

Ab initio total energy calculations, based on the exact muffin-tin orbital (EMTO) theory, were used to determine the **elastic properties of $Al_{1-x}Li_x$ random alloys** (x<0.20) in the face centered-cubic crystallographic phase. The compositional disorder was treated within the framework of the single-site coherent potential approximation (CPA), whereas the effect of the local lattice relaxation on the elastic constants was estimated using a supercell technique. We have found that the calculated equilibrium volumes and alloy formation energies strongly depend on the approximations employed in the Poisson equation, in accordance with former observations. At the same time, the experimental trends of the elastic moduli of disordered Al-Li alloys are well reproduced by the EMTO-CPA method. Using our theoretical results we have shown that the nonlinear effect of Li addition on the elastic constants originates from the detailed band structure of Al near the Fermi level.

The high-pressure equation of state and **elastic properties of solid He^4** have been calculated using density functional theory formulated in the framework of the exact muffin-tin orbitals method. The theoretical results, obtained within the generalized gradient approximation for the exchange-correlation functional, are in good agreement with the experimental data available for pressures between 13 GPa and 32 GPa. We predict that at 0 K the hexagonal phase of He remains mechanically and thermodynamically stable up to the highest pressure considered in the present study (150 GPa). The calculated anisotropy ratios of He are similar to those observed in the case of hexagonal metals with c/a~1.63. On the other hand, we find that hydrostatic pressure has negligible effect on the anisotropy of He. This indicates that He can be used as a quasihydrostatic medium in high-pressure experiments up to at least 150 GPa.

An efficient procedure to calculate **surface segregation profiles** of substitutionally disordered binary alloys is presented. We show that a simple thermodynamic model with realistic atomic configurations at the surface region combined with the total energies obtained from exact muffin–tin orbitals calculations leads to accurate surface segregation profiles. We find that the calculated surface segregation energies in random alloys show significant dependence on the local environment of the atoms involved in the segregation process. Correspondingly, the alloy surface energy is significantly affected by the subsurface atomic layers. As an example the PdAg(111) surface is considered.

Iron and magnesium are almost immiscible at ambient pressure. The low solubility of Mg in Fe is due to very large size mismatch between the alloy components. However, the compressibility of Mg is much higher than that of Fe, and therefore the difference in atomic sizes between elements decreases dramatically with pressure. Based on the predictions of *ab initio* calculations, we demonstrate in series of experiments in a multianvil apparatus and in electrically- and laser-heated diamond anvil cells, that high pressure promotes solubility of magnesium in iron. At megabar pressure range more than 10 at% of Mg can be dissolved in Fe and then quenched to ambient conditions. Study of the equation of state of low Mg-concentration iron-magnesium alloy suggests that the difference in densities of pure iron and 4.1 at% Mg-Fe alloy comes mainly from the difference in atomic masses in agreement with theoretical predictions. A generality of the concept of **high-pressure alloying between**

[+] Permanent position: Budapest University of Technology and Economics

immiscible elements is demonstrated by its application to two other Fe group elements, Co and Ni.

Currently we are engaged in large calculations on the **magneto-crystalline anisotropy of surface nanostructures**. We are performing a comprehensive study for various geometries of different kinds of magnetic atoms on a variety of substrates. This data is of utmost importance for the design of ultra-high-density magnetic recording devices.

We carried out a **symmetry analysis** of the so-called hidden order of the T<17K phase **of URu_2Si_2.** Ruling out dipoles and quadrupoles, we showed that available experimental evidence is compatible with octupolar order. Furthermore, we analyzed the possibilities of a second symmetry breaking transition occurring on the background of pre-existing octupolar order. We showed that the recently observed T=13.5K NQR anomaly can be interpreted as evidence of quadrupolar order accompanied by a new time reversal invariance breaking order which may be either dipolar, or octupolar, or of triakontadipole character .

We discussed the **anisotropy of the spin susceptibility** of the correlated transition metal sulphide $BaVS_3$. In cooperation with the group of Prof. L. Forró (Lausanne, Switzerland), we analyzed ARPES data on $BaVS_3$ and showed that its behavior is controlled by the overlap of wide a_{1g} and narrow e_g d-bands.

Using the density functional theory formulated within the framework of the exact muffin-tin orbitals method, we have made a systematic study of the top **layer relaxation and surface stress** of 4d transition metals. Our calculations predict layer contractions for most surfaces. We have found that the relaxations of the close packed surfaces decrease with increasing atomic number through the 4d series. We propose that the relaxation is mainly due to the reduction of the number of sp electrons in the surface layer relative to bulk. The surface stress is found to be very sensitive to the relaxation and, therefore, an accurate determination of the layer relaxation is necessary for obtaining reliable values for the surface stress. Comparing the top layer relaxations for the close packed surfaces, we see essential deviations between data derived in different ab initio calculations. At the same time, the overall trend for our calculated surface stress of 4d metals is in reasonable agreement with recent full-potential data.

We have continued to investigate some special transport properties of **unconventional density waves** (UDW) in quasi one, and two dimensional systems. Our calculations of the angular dependent magnetoresistance (ADMR), the magnetothermopower (MTP) and the Nernst effect indicate that UDW may be responsible for the observed experimental behavior in the pseudogap phase of some underdoped high-T_c cuprates like LSCO and YBCO, and in the heavy fermion material $CeCoIn_5$. We have studied the effect of imperfect nesting on the density of states and optical conductivity of UDW. We gave a comprehensive account of the Raman spectra in UDW in various scattering geometries, and considered collective contributions as well. We pointed out, that the amplitude mode of the UDW is overdamped due to decay into the quasiparticle continuum.

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Grants and international cooperations

OTKA T048827 First principles calculations for surfaces; surface stress and segregation (J. Kollár, 2005-2008)
TÉT SF-15/03 (Hungarian-Finnish) Quantummechanical modelling of structural electronic and magnetic properties of alloy surfaces (J. Kollár, 2004-2005)
EFS Programme: Toward atomistic materials design (J. Kollár, 2003-2007)
OTKA 46773 Investigation of metals and alloys by density functional theory (L. Vitos, 2004-2007)
HAS-JSPS (Hungarian-Japanese bilateral) Competition and frustration in multipolar ordering phenomena (P. Fazekas, 2003-2005)

Publications

Articles

C.1. Korzhavyi* PA, Vitos L, Andersson* DA, Johansson* B; Oxidation of plutonium dioxide; *Nature Materials*; **3**, 225-228, 2004

C.2. Punkkinen* MPJ, Vitos L, Kokko* K, Laaksonnen* K, Väyrynen* IJ; Electronic and magnetic properties of bulk and (100) and (111) surfaces of the $MnPt_3$: An *ab initio* study; *Phys Rev B*; **70**, 024411/1-6, 2004

C.3. Vitos L, Korzhavyi* PA, Johansson* B; Austenitic stainless steels from quantum mechanical calculations; *Advanced Engineering Materials*, **4**, 228-232, 2004

C.4. Magyari-Köpe* B, Vitos L, Grimvall* G; Anomalous behavior of lattice parameters and elastic constants in hcp Ag-Zn alloys; *Phys Rev B*; **70,** 052102/1-4, 2004

C.5. Landa* A, Sönderlind* P, Ruban* A, Vitos L, Pourovskii* L V; First-principles phase diagram for Ce-Th system; *Phys Rev B*; **70**, 224210/1-5, 2004

C.6. Sönderlind* P, Landa* A, Sadigh* B, Vitos L, Ruban* A; First-principles elastic constants and phonons of δ-Pu; *Phys Rev B*; **70**, 144103/1-5, 2004

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D. NON-EQUILIBRIUM ALLOYS

I. Vincze, J. Balogh, L. Bujdosó, D. Kaptás, T. Kemény, L.F. Kiss

Incommensurate antiferromagnetism in $FeAl_2$. — The research of the magnetic properties of *bcc* Fe-Al alloys is since long in the center of interest because of the simple atomic structure and the complicated, spin glass-like magnetic behaviour following ferromagnetism above 30 at.% Al content. Often believed that antiparallel Fe magnetic moments based on an early hypothesis of antiferromagnetic Fe-Al-Fe superexchange may explain the magnetic anomalies. However, FeAl is nonmagnetic and no unambiguous evidence was found for the existence of oppositely oriented magnetic moments in the Fe-Al system.

In $FeAl_2$ unambiguous evidence is given for the existence of antiferromagnetically coupled Fe magnetic moments on the base of Mössbauer and magnetization measurements.

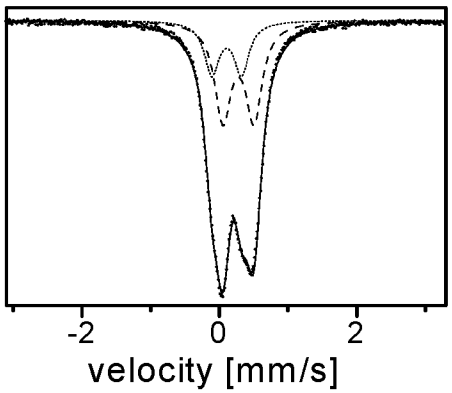

Fig. 1: *Room temperature Mössbauer spectrum of $FeAl_2$. Full line is the fitted curve consisting of two quadrupole doublet, the Fe_h and the Fe_l components are marked by the dotted and broken lines, respectively.*

The room temperature Mössbauer spectrum is shown in Fig. 1. It shows clearly the presence of two iron environments, designated as Fe_h and Fe_l with no detectable amount of disorder (*i.e.* no line broadening is observed). The relative occupation of the two sites was found to be Fe_h:Fe_l =1:2. If we assume a close packed structure our data suggest that the Fe_h atoms have about 6±1 Fe and the Fe_l atoms have about 3±1 Fe nearest neighbours, respectively.

The Mössbauer spectrum measured at 4.2 K is shown in Fig. 2a. Here the two Fe sites are also clearly distinguishable: the site denoted by Fe_h has the larger hyperfine field. The lines are structureless and quite broad, individual hyperfine field values cannot be resolved, only the hyperfine field distribution shown in Fig. 2b can be determined. Two peaks can be distinguished in the hyperfine distribution as shown in the figure, the ratio of the respective areas under the subdistributions is 2:1 as for the quadrupole doublets in the room temperature paramagnetic spectrum. The average values of these subcomponents are B_h = 11.3 T and B_l = 4.8 T, respectively. These values are related to the values of the individual Fe magnetic moments. In close packed intermetallic compounds the neighbour contribution is less than 10% and the Fe hyperfine field is in good approximation proportional to the Fe magnetic moment with a proportionality

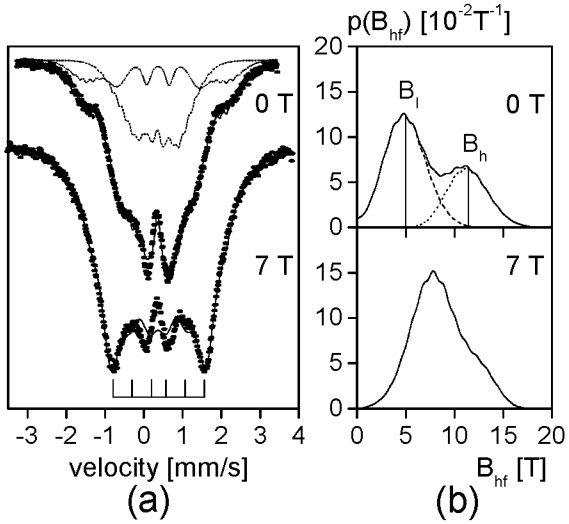

Fig. 2: *Mössbauer spectra of $FeAl_2$ at 4.2 K (a) and the respective Fe hyperfine field distributions (b) in 7 T and without applied magnetic field, full lines are the fitted curves. The components of the Fe_h and Fe_l environments are shown as the dotted and broken lines, respectively. In 7 T the comb shows the positions of the six-line pattern of the average hyperfine field.*

constant of 13 T/μ_B. This assumption would give about 0.9 μ_B and 0.4 μ_B for the iron magnetic moments in the Fe-rich and Fe-poor environments, respectively.

The Mössbauer spectrum measured at 4.2 K in B_{ext} = 7 T external magnetic field is shown in Fig. 2b. The shapes of the spectra are considerably different in B_{ext} = 0 and 7 T: it is clear that the second and fifth lines did not disappear (i.e. $I_{2,5} \neq 0$) and a small increase (about 1.3 T) in the average hyperfine field is observed. The shape of the hyperfine field distribution and the value of $I_{2,5}$ is strongly correlated, thus the hyperfine field distribution shown in 7 T (Fig. 2b) has large systematical uncertainty. It is clear, however, that the most significant difference with respect of the 0 T distribution is the broadening of the low field part of the distribution and some decrease in the intensity of the second and fifth lines of the spectra. The components with increased hyperfine field are infallible finger-prints of antiferromagnetically oriented Fe magnetic moments.

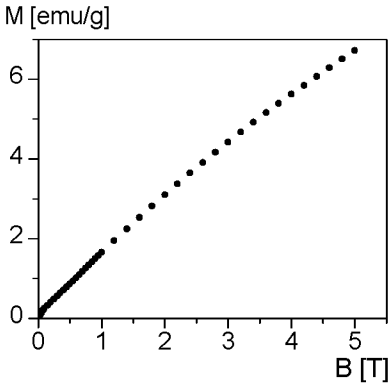

Fig. 3: *The applied magnetic field dependence of the magnetization measured at 5 K.*

The magnetization measured at 5 K up to 5 T is shown in Fig. 3. It is almost linear as the function of the applied field, which means a complete compensation of the magnetic moments and very strong magnetic anisotropy.

Neutron diffraction measurements of E. Sváb, Z. Somogyvári and G. André at 1.5 K performed in LLB, Saclay show the presence of magnetic satellites which correspond to an incommensurate magnetic structure with a periodicity of about 1.1 nm.

Fe/Ag granular multilayers and heterostructures. — Control over the shape, size and spacing of the magnetic elements in nanoscale composites is an important issue, not only for applications, but also for our basic understanding of the interactions among magnetic elements. We demonstrated two interesting properties of Fe-Ag granular multilayers:

(i) The magnetic grain size can be reduced not only by decreasing the thickness of the magnetic layers (d_{Fe}), but also by increasing the Ag layer thickness (d_{Ag}).

(ii) Continuous magnetic layers can be inserted into the granular multilayer structure without modifying the average magnetic grain size (derived from the superparamagnetic blocking temperature (T_B)) and the almost perpendicular magnetic alignment of the granular layers.

The possibility of control over the superparamagnetic grain size, the amount and the stacking sequence of the ferromagnetic fraction makes these heterostructures suitable model materials for understanding the magnetic behavior of granular composites with randomly distributed magnetic elements. Comparing SQUID magnetization and Mössbauer measurements we have found that varying the stacking sequence affected the low field magnetic susceptibility of the ferromagnetic layers more significantly than that of the superparamagnetic ones.

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Grants and international cooperations

OTKA T 048965	Magnetic properties of multilayer structures (J. Balogh, 2005-2008)
OTKA T038383	Interaction of superparamagnetic clusters (L.F. Kiss, 2002-2005)
OTKA T046795	Superferromagnetism in nanostructures (I. Vincze, 2004-2007)

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D.7. Kaptás D, Sváb E, Somogyvári* Z, André* G, Kiss LF, Balogh J, Bujdosó L, Kemény T, Vincze I; Incommensurate antiferromagnetism in $FeAl_2$: magnetic, Mössbauer and neutron diffraction measurements; *Phys Rev B*; accepted for publication

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See also E.22., H.3., H.4., K.18.

E. X-RAY DIFFRACTION

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Fullerenes and related systems. — The fullerenes are closed shell all carbon atom molecules. The most abundant among them is the C_{60} molecule.

Fullerenes can form a large variety of compounds with elements or with other molecules. In the group of A_xC_{60} compounds (A=Na, K, Rb, Cs) there are materials with very interesting properties. Many superconducting materials (A_3C_{60}), and also polymers with different dimensionality (RbC_{60}, Na_4C_{60}) were found. We studied the infrared, optical and neutron scattering spectra of the 2D alkali fulleride salt A_4C_{60}. We detected the transition between static and dynamic Jahn-Teller effect in these compounds on changing the temperature. These experiments are among the first evidences of the Mott-Jahn-Teller nonmagnetic insulating state in fullerides.

Similarly to fullerenes cubane (C_8H_8) is also a cage-molecule. We successfully synthesized high symmetry molecular crystals from C_{60} and C_{70} with cubane. It was shown that the two type of molecules form crystals as a result of molecular recognition between the convex surface of fullerenes and the concave cubane. Static cubane occupies the octahedral voids of the face centered cubic structures and acts as a bearing between the rotating fullerene molecules. The smooth contact of the rotor and stator molecules decreases significantly the temperature of orientational ordering. These novel materials have great topochemical importance: at elevated temperatures they transform to high stability covalent derivatives while preserving their crystalline appearance. The size-dependent molecular recognition promises selective formation of related structures with higher fullerenes and/or substituted cubanes.

Similarly to the fullerene molecules, carbon nanotubes are also exclusively built from carbon atoms. We have developed methods for preparing thin carbon nanotube layers on various substrates and also freestanding thin films. We modeled the optical properties of these layered structures and studied the effects of ionic doping on the optical spectra. We extended our optical investigations to oriented carbon nanotube samples in polarized light.

Ab initio structure solution – In previous years we have developed an iterative structure solution algorithm, termed charge flipping. It works ab initio on high-resolution x-ray diffraction data in the manner of Fourier recycling. The original scheme explores the high-dimensional space of structure factor phases mainly in real-space: in each cycle the sign of electron density below a threshold is reversed. Recently, we have found an efficient modification of the algorithm that complements the phase exploration in reciprocal-space. Before starting the iteration process measured intensities are sorted, and a fraction of reflections are marked as weak. Strong reflections are used as before: only their observed moduli are prescribed. Weak reflections are treated in a new way: their calculated moduli are accepted unchanged and calculated phases are shifted by the constant $\pi/2$. This means that observed data of these reflections are not used in the iteration, except for the knowledge that they are indeed weak. The improvement is drastic, in some cases the success rate is increased by a factor of ten, in other cases a previously unsolvable structure becomes solvable by the modified algorithm. Paradoxically, it is better not to use observed moduli of

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weak reflections, in the search for a solution they create only unwanted constraints. Practical applications of the charge flipping method are already appearing in the literature. Because the algorithm is not based on atomicity, it is excellently suited to the solution of modulated structures, for which no other direct methods exist.

Theory of phase transformations. — A phase field theory of polycrystalline solidification has been developed that is able to describe the nucleation and growth of anisotropic particles with different crystallographic orientations in three dimensions. As opposed with the two-dimensional case, where a single orientation field suffices, in three dimensions, minimum three fields are needed. The free energy of grain boundaries has been assumed to be proportional to the angular difference between the adjacent crystals, which has been expressed here in terms of the differences of the four symmetric Euler parameters. The equations of motion for these fields have been obtained from variational principles. Illustrative calculations were performed for polycrystalline solidification with dendritic, needle and spherulitic growth morphologies (Fig. 1).

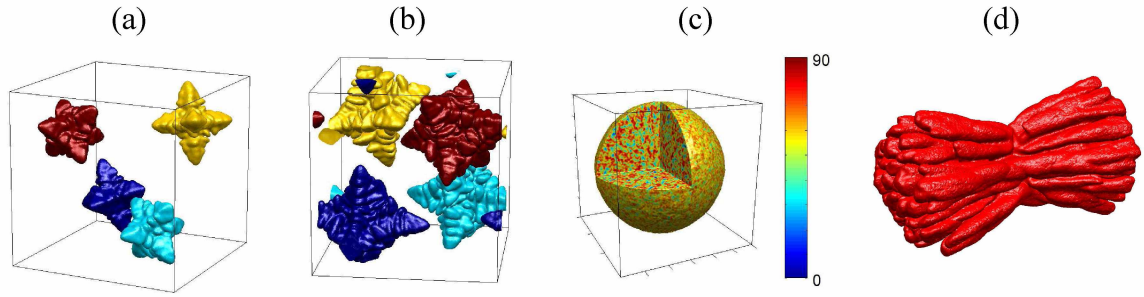

Figure 1. Polycrystalline freezing in three dimensions: (a), (b) Snapshots showing the growth of four randomly oriented dendrites assuming cubic crystal symmetry (400×400×400 grid). Note the effect of periodic boundary conditions: The branches that grow out of the simulation on one side of the simulation box, enter on the opposite side. (c) Polycrystalline spherulite formed by trapping of orientational disorder calculated triclinic crystal symmetry (300×300×300 grid). (d) A crystal sheaf formed by branching of a needle crystal simulated with triclinic crystal symmetry (250×250×500 grid; with an ellipsoidal symmetry of the phase field mobility). The $\phi = 0.5$ surface is shown.

A phase-field theory of binary liquid phase separation coupled to fluid flow has been developed. The respective Cahn-Hilliard-type and Navier-Stokes equations have been solved numerically. We incorporated composition and temperature dependent capillary forces. The free energies of the bulk liquid phases were taken from the regular solution model. In the simulations, we observed Marangoni motion, and direct and indirect hydrodynamic interactions between the droplets. We have found that coagulation is dramatically accelerated by flow effects.

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Grants and international cooperations

OTKA T049338 Optical spectroscopy of molecular carbon structures (K. Kamarás, 2005-2008)

GVOP-3.2.1.–2004–04–0009/3.0 Acquisition of far-infrared spectrometer (K. Kamarás, 2005-2006)

GVOP-3.2.1.–2004–04–0008/3.0: Analitical applications and development of STM and AFM (G. Faigel, 2005-2006)

OTKA T043237 Elastic x-ray scattering in structural research (G. Faigel 2003-2006)

OTKA T 048298 Holographic methods in structural research (M. Tegze, 2005-2008).

OTKA T037323 Dynamics of non-equilibrium morphologies (L. Gránásy, 2002-2005).

ESA PECS 98005 Phase field modeling of magnetic and composite materials (L. Gránásy, 2004–2006)

ESA PECS 98021 Phase field modeling of solidification in monotectic systems (L. Gránásy, 2004–2006)

Participation in EU FP6–500635-8 project, IMPRESS Intermetallic Materials Processing in Relation to Earth and Space Solidification (L. Gránásy, 2004–2009)

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See also D.2., H.10., H.11.

F. ELECTRON CRYSTALS

G. Kriza, P. Matus[#], Gy. Mihály[+], L. Németh[#], Á. Pallinger[#], B. Sas, F.I.B. Williams

Dissipation in high-T_c superconductors. — Vortices in the high-T_c superconductor $Bi_2Sr_2CaCu_2O_8$ (BSCCO) at low temperature and high field form a stack of quasi 2-D solids pinned to the host disorder with little correlation from plane to plane. Subjected to a sufficiently strong transport supercurrent, they depin bringing into play dissipative forces. The simultaneous appearance of a potential drop transverse to the current flow indicates that their motion is not perfectly orthogonal to the current, but the fact that it is identical for oppositely directed fields indicates that it is not a true Hall effect such as might be expected to arise from free flux flow. It is rather taken to indicate channeling along paths determined by the random pinning potential of the host. Up to now no real Hall effect (defined by a part of the transverse potential antisymmetric in magnetic field) has ever been detected in this solid phase. Very recently, with our newly developed shorter and higher intensity pulse electronics (up to 1.2 A and down to 1 μs), we have observed for the first time a bifurcation in the transverse $E - I$ response between positively and negatively directed magnetic fields at currents two orders of magnitude higher than the initial depinning threshold in a low threshold underdoped sample ($T_c \approx 53$ K). This appearance of a Hall effect is interpreted as dechanneling and a change of regime towards non-constrained flux flow. We believe this newly observed phenomenon to be a manifestation of the transverse rigidity of conduction channels proposed theoretically by Giamarchi and Le Doussal and seen up to now in the magnetically induced Wigner solid only.

In view of the importance and first ever nature of these results, the experiments require careful confirmation and checks on their universality. It is to be hoped that development of these experiments will also allow an indication on the reordering of the solid expected to occur beyond a certain vortex lattice velocity.

Nuclear magnetic resonance in correlated electronic systems. — We have investigated the ^{77}Se NMR properties of single crystals of $(TaSe_4)_2I$. This is a quasi-one-dimensional compound with charge density wave (CDW) ground state. The high-temperature "normal" phase shows signs of a depleted density of states at the Fermi level, a phenomenon referred to as "pseudogap." The pseudogap phenomenon is also found in underdoped samples of high-temperature superconductors and is therefore of great interest. We have compared several classes of density-of-states functions to our NMR Knight shift and spin-lattice relaxation rate data and found that only models with a true gap are able to reproduce simultaneously these two NMR parameters. The existence of a true gap in the normal state indicates a hidden order parameter and contradicts the conventional interpretation of the pseudogap phenomenon based on fluctuating CDW order. Signs of critical fluctuations at the CDW transition are absent in our spin-spin relaxation time data in agreement with a first order transition in contrast to the second order transition predicted by conventional theory.

Installation of new equipment. — As a part of an ongoing collaboration agreement with the *Service de Physique de l'Etat Condensé* (SPEC) at the CEA-Saclay, France, equipment has been installed which opens up new possibilities in the realm of vortex and electron transport and microwave spectroscopy to very low temperatures and high magnetic fields. This equipment includes a ^{3}He/^{4}He dilution refrigerator inserted into a superconducting

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magnet and a swept-frequency microwave spectrometer suitable for measurements at millikelvin temperatures.

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Grants and international cooperations

OTKA T037976	Dissipation in type-II superconductors (G. Kriza, 2002-2005)
OTKA TS040878	Collective electronic states in solids (G. Kriza, 2002-2005)
SPEC – Saclay	Collaboration agreement with Service de Physique de L'Etat Condensé (SPEC) CEA-Saclay, France on electron crystals and nano-electronics (2005-2008)

Publications

Articles

F.1 Matus P, Alloul* H, Singer* PM, Brouet* V, Kriza G, Garaj* S, Forró* L; Fullerene local order in Na_2CsC_{60} by ^{23}Na NMR; *Appl Magn Res;* **27**, 133-138, 2004

F.2 Nándori* I, Vad* K, Mészáros* S, Hakl* J, Sas B; Length-scale dependence in layered superconductors; *Czech. J Phys*; **54**, Suppl. D, D481-D484, 2004

F.3 A. Beya-Wakata* A, Hennigan* PF, Gaal R, Mellor* CJ, Williams FIB, Henini* M; Microwave resonance susceptibility of a two-dimensional hole system in a weak random potential; *Phys Rev B*; **71**, 235319/1-7, 2005

F.4 Vad* K, Mészáros* S, Sas B; Transverse and secondary voltages in $Bi_2Sr_2CaCu_2O_8$ single crystals; *Physica C;* **432**, 43-52, 2005

F.5 Matus P, Alloul* H, Kriza G, Brouet* V, Singer* PM, Garaj* S, Forró* L; NMR evidence for C_{60} configurational fluctuations around Na sites in Na_2CsC_{60}; *J Superconductivity;* accepted for publication

See also: E.9., E.12, E.22.

G. LIQUID CRYSTALS

Á. Buka, T. Börzsönyi, N. Éber, K. Fodor-Csorba, A. Jákli, I. Jánossy, T. Tóth-Katona, A. Vajda

A detailed theoretical and experimental analysis of the ***decay of periodic roll patterns*** was carried out in a planarly aligned nematic liquid crystal. The relaxation time was measured as a function of the wave number of the pattern using a light diffraction technique. A theoretical analysis explored a rich structure of dispersion curves for the decay rates. An interesting relation was found between the realistic case of no-slip boundary conditions and the simpler free-slip case. The experimentally determined decay rates, both for "conductive" and for "dielectric" initial patterns, followed the theoretical solution with subsequent jumps between branches when the wave number was increased.

A nematic liquid crystal composed of ***bent-core molecules*** synthesized in our laboratory showed fascinating patterns in electric field (see e.g. the 'knitting' instability in Figure 1). An important attribute of this material is that the anisotropy of the electrical conductivity changes sign twice as the frequency of the applied electric field is increased. Three ***nonstandard electro-hydrodynamic instabilities*** were detected and characterized, which did not appear to fit within the standard model for electroconvection. The first instability (at lowest frequencies) created a pattern with stripes parallel to the initial director orientation, with a wavelength about equal to the separation of the cell plates. The other two corresponded to the prewavy instability. They both had the same optical appearance and dynamical characteristics, but could be distinguished by their frequency range and by different threshold behaviour.

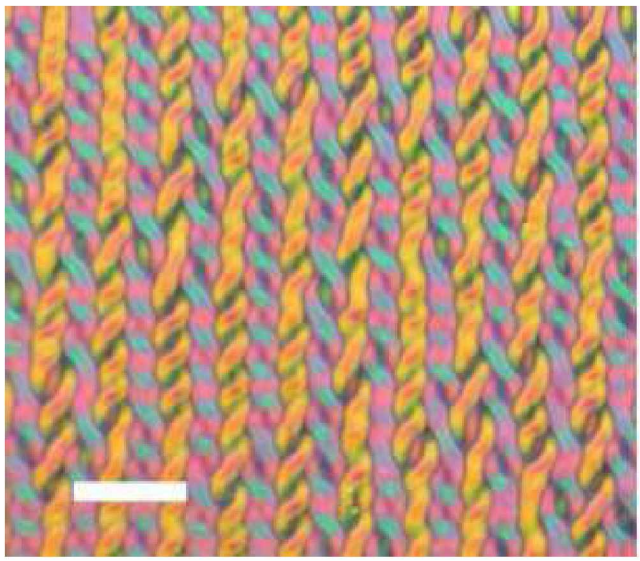

Figure 1. The "knitting" instability in the bent-core nematic at 40 kHz and 35 V_{rms} produced by abruptly raising the voltage from one of the prewavy states (viewed at crossed polarisers). The length scale (white rod) represents 100 μm.

The liquid crystalline homologoues series of 4-(alkoxyphenyl) cubane-1,4-dicarboxylates, prepared in the previous year, were transformed into cuneane-caged derivatives by a catalytical rearrangement reaction. The homologoues series of 4-n-(alkoxyphenyl) cuneane-1,4-dicarboxylates (see one representative in Figure 2) are the first ***cuneane-caged liquid crystals.*** They exhibit nematic and SmA phases.

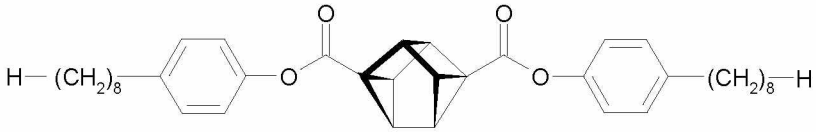

Figure 2. Chemical formula of the 4-n-(octyloxyphenyl) cuneane-1,4-dicarboxylate

Though formation of ten isomers is theoretically expected for the rearrangement reaction, only two of them (Figure 3) were actually detected. The ratio of the 1,3-cuneane- and 2,6-cuneane-dicarboxylate derivatives was 1: 9 according to NMR spectroscopy and HPLC.

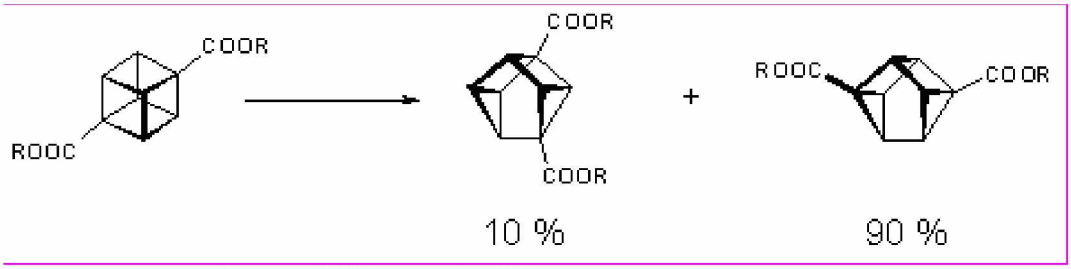

Figure 3. The result of the rearrangement reaction

Swelling properties of self-standing, isotropic ***elastomer*** films (prepared through a cross-linking process of prepolymer components) were characterised in various solvents. Magnetic nanoparticles from colloidal suspensions were efficiently incorporated in the urethane/urea elastomer by swelling the samples with a toluene and ferrofluid mixture. The ratio of birefringence to strain was found greater in the ferrofluid-doped samples than in the pure elastomer samples, indicating that ferrofluid grains became oriented by the strained polymer network.

Our recent studies in ***granular systems*** indicated that varying the grain shape might result in a strong change in the dynamics (e.g. avalanche propagation). A high speed video imaging system is developed for the experimental investigations of these dynamical processes of granular materials.

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Grants and international cooperations

OTKA T037275 Interaction of liquid crystals and polymer films (I. Jánossy, 2002-2006)

OTKA T-037336 Flow phenomena in liquid crystals (N. Éber, 2002-2006)

MTA-OTKA-NSF Investigation of liquid crystalline mesophases of bent core molecules (Á. Buka, 2002-2005)

MTA-INSA (Hungarian-Indian bilateral) Experimental and theoretical studies on liquid crystals (N. Éber, 2004-2006)

MTA-CAS (Hungarian-Chinese bilateral) Physical and chemical study of liquid crystals (N. Éber, 2004-2006)

MTA-SASA (Hungarian-Serbian bilateral) Structure and physical study of liquid crystals (N. Éber, 2004-2006)

MTA-WATWAW (Hungarian-Polish bilateral) Study of liquid crystals (K. Fodor-Csorba, 2004-2006)

MTA-ASCR (Hungarian-Czech bilateral) Synthesis and study of ferroelectric liquid crystals leading to preparation of mixtures with defined properties (K. Fodor-Csorba, 2004-2006)

MTA-CNR (Hungarian-Italian bilateral) New banana-shaped monomers and their polymer derivatives (K. Fodor-Csorba, 2004-2006)

EU-HPCF-CT-2002-00247 Nonequilibrium in physics and in biology (Á. Buka, 2002-2005)

EU-HPRN-CT-2002-00312 Nonequilibrium physics from complex fluids to biological systems (Á. Buka, 2002-2006)

EU-MSCF-CT-2004-013119 Interactive training and research in nonlinear science from physics to biology (Á. Buka, 2004-2008)

PST.CNS 975474 NATO linkage grant Patterns and chaos in electroconvection of liquid crystals (Á. Buka, 2000-)

56ÖU4 Austrian-Hungarian Action Foundation. Polymers made of Banana-molecules – How to conserve unique properties (K. Fodor-Csorba, 2004-March 2005)

Long term visitors

— David Statman: Alleghiny College, Meadville, Pennsylvania, USA, 15 June-15 July, 2005, (host: I. Jánossy).

— Vincent Werner: Alleghiny College, Meadville, Pennsylvania, USA, 15 June-15 July, 2005, (host: I. Jánossy).

— K.L. Sandhya: Centre for Liquid Crystal Research, Bangalore, India, June-August 2005, (host: I. Jánossy).

— Aude Cauquil-Vergnes: University of Montpellier, Montpellier, France, 1 January-30 July, 2005, (EU-RTN grant, host: Á. Buka).

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Articles

G.1. Éber N, Rozanski* SA, Németh Sz, Buka Á, Pesch* W, Kramer* L; Decay of spatially periodic patterns in a nematic liquid crystal; *Phys Rev E;* **70,** 061706/1-8, 2004

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G.4. Bényei* Gy, Jalsovszky* I, Slugovc* C, Trimmel* G, Pelzl* G, Vajda A, Éber N, Fodor-Csorba K; Structure and properties of new liquid crystalline cubane-1,4-dicarboxylic acid derivatives; *Liquid Crystals;* **32**, 197-205, 2005

G.5. Xu* J, Fodor-Csorba K, Dong* R; Orientational order of a bent-core mesogen by two dimensional ^{13}C NMR spectroscopy; *J Phys Chem A;* **109**, 1998-2005, 2005

G.6. Jánossy I; High-precision measurement of azimuthal rotation of liquid crystals on solid substrates; *J Appl Phys;* **98**, 043523/1-6, 2005

G.7. Éber N, Buka Á; Electroconvection in homeotropic nematic liquid crystals; *Phase Transitions;* **78**, 433–442, 2005

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G.9. Börzsönyi T, Halsey* TC, Ecke* RE; Two scenarios for avalanche dynamics in inclined granular layers; *Phys Rev Lett;* **94**, 208001/1-4, 2005

G.10. Barmatov* E, Calucci* L, Catalano* D, Chiezzi* L, Veracini* CA, Fodor-Csorba K; ^{2}H-NMR of the Induced Chiral Phases of Acrylate-Metacrylate Liquid Crystalline Copolymers; *Mol Cryst Liq Cryst*; **429**, 181-191, 2005

G.11. Kochowska* E, Éber N, Otowski* W, Buka A; Square patterns and their dynamics in electroconvection; *Mol Cryst Liq Cryst;* **435**, 243-253, 2005

G.12. Galli* G, Demel* S, Slugovc* C, Weissflog* W, Diele* S, Fodor-Csorba K; Novel liquid crystal ADMET polymers with main chain mesogens; *Mol Cryst Liq Cryst;* **439**, 1909-1919, 2005

G.13. Otowski* W, Biernat* A, Fodor-Csorba K, Witko* W; Spectroscopic investigation of ferroelectric liquid crystals composed of banana-shaped achiral molecules; *Mol Cryst Liq Cryst*, accepted for publication

G.14. Obadović* DZ, Vajda A, Garić* M, Bubnov* A, Hamplová* V, Kašpar* M, Fodor-Csorba K; Thermal analysis and X-ray studies of chiral ferroelectric liquid crystalline materials and their binary mixtures; *J Thermal Analysis and Calorimetry;* accepted for publication

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G.15. Bényei* G, Jalsovszky* I, Fodor-Csorba K; Structure property relationship study on new cubane-1,4-dicarboxylic acid derivatives; In: *XV. CLC Conference 13-17 October 2003, Zakopane, Poland*; Ed.: J. Zmija, Proc. SPIE. **5565**; pp. 6-12, 2004

G.16. Buka Á, Éber N, Pesch* W, Kramer* L; Convective patterns in liquid crystals driven by electric field. An overview of the onset behavior; In: *Self-Assembly, Pattern Formation and Growth Phenomena in Nano-Systems, St. Etienne, France, August 2004;* Ed.: A. Golovin, NATO ASI series, Kluwer Academic Publishers; accepted for publication

See also: E.19., E.23., E.27.

H. METAL PHYSICS

K. Tompa, I. Bakonyi, P. Bánki, M. Bokor, Cs. Hargitai, Gy. Lasanda, L. Péter, J. Tóth, E. Tóth-Kádár

Metal-hydrogen systems. — High purity Pd and $Pd_{1-x}Ag_x$ (x = 0.1; 0.2 and 0.35) alloys were charged with hydrogen, and ^{1}H NMR free induction decay and different echoes were measured down to 2.4 K on this fcc crystalline alloy, on a model material representing a chemically disordered system for the hydrogen storage materials. Samples of H/M = 0.04 hydrogen content were prepared and investigated. In the very low temperature range (2-3 K) inhomogeneous echoes were detected near the commonly known solid echoes, suggesting a strong paramagnetic contribution to the proton NMR spectrum. An unambiguous correlation was found between the magnetic susceptibility and the NMR line width of the inhomegeneous echoes (Fig. 1) The substantial deviation from this rule at the 25% Ag containing alloy is a consequence of the high Fe impurity content of the sample.

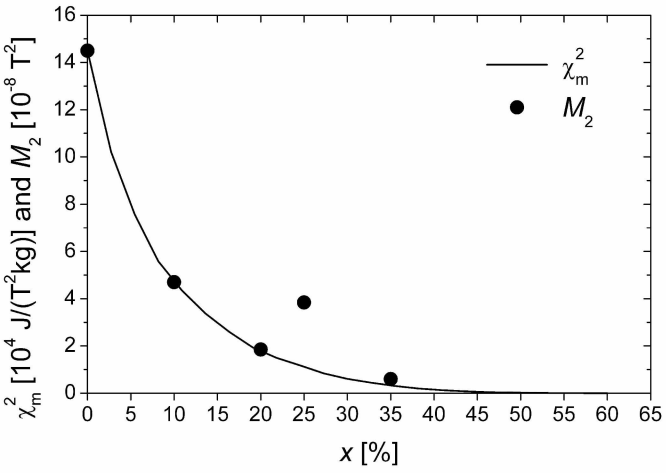

Figure 1.

Magnetic susceptibility squared and the second moment of inhomogeneous echo as a function of silver content.

Carbon materials – fullerene-cubane. — The results of ^{1}H NMR measurements verified that the cubane molecules are static in the crystal lattice of the $C_{60}{\cdot}C_8H_8$ compound. This statement is supported by the following arguments. (a) The ^{1}H NMR spectrum remains unchanged in the studied wide temperature range of 130 to 381 K and is independent of the magnitude of the applied radiofrequency field. (b) The spectrum has a definite fine structure resembling a shape expected for a static multi-spin system (Fig. 2). The onset of reorientation would cause severe narrowing (by one order of magnitude) and loss of structure in the spectrum. (c) The measured second moment of the spectrum agrees excellently with the calculated value for static cubane molecules. Reorientation of the cubane molecules would result

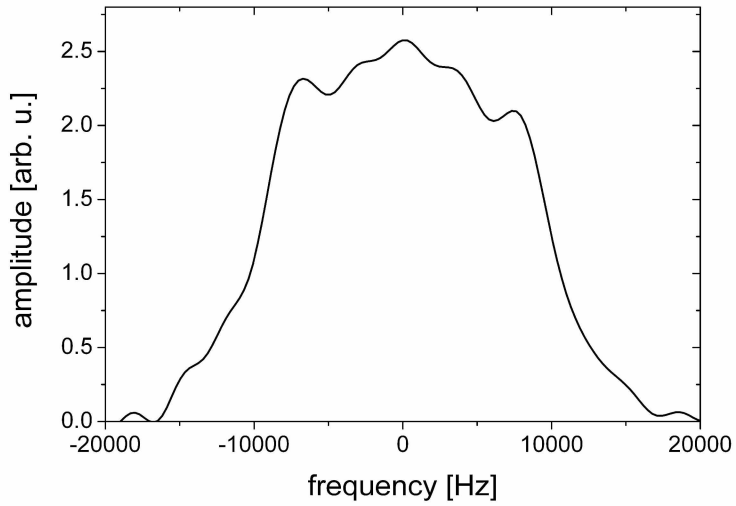

Figure 2. ^{1}H NMR spectrum for $C_{60}{\cdot}C_8H_8$ at T = 130 K and ν_0 = 82.467 MHz

in a second moment reduced by a factor of 50.

Hydration of semi-structured proteins. — The temperature dependence of NMR Free Induction Decay (FID) signal amplitude of water protons together with DSC (differential scanning calorimetry) were measured in physiological solutions of semi-structured proteins, namely ERD-10 and as a reference material of structured (globular) protein BSA, moreover in the buffer and NaCl solutions. Different aspects of protein-buffer (and protein-NaCl) interaction were detected microscopically by NMR and thermally by DSC. The quantitative characteristics of the interaction are different for the semi-structured ERD-10 and for the gobular BSA. The hydration number with respect to an amino acid is about 2.5 times higher in ERD-10 than in BSA. (The work is carried out in cooperation with the Institute of Enzymology, Biological Research Center, HAS).

Atomic volumes and local structure of metallic glasses. — The composition dependence of the room-temperature average atomic volume derived from published density data was analysed for early and late transition metal (TE-TL type) and metal-metalloid (TL-MD type) amorphous alloys. For the Zr-Cu, Ti-Cu and Hf-Ni sytems, the data suggest an ideal solid solution behaviour. For the other TE-TL systems, two composition ranges can be distinguished (range 1: 20 to 70 at.% TL; range 2: 84 to 93 at.% TL). For each composition range, a specific atomic volume $V_{a\text{-}Zr}$ can be assigned to the Zr atoms that has the same value for any of the alloying components TL = Fe, Co and Ni. For TE-rich compositions, $V_{a1\text{-}Zr} \approx V_{hcp\text{-}Zr}$ whereas for TL-rich compositions, $V_{a2\text{-}Zr} < V_{a1\text{-}Zr}$. For the TL atoms, whereas both $V_{a2\text{-}TL}$(TE-TL) and $V_{a\text{-}TL}$(TL-MD) are fairly close to the V_{TL} values of the corresponding close-packed crystalline structures, the $V_{a2\text{-}TL}$(TE-TL) values are smaller by as much as about 10 % than the $V_{a\text{-}TL}$(TL-MD) values.

GMR in electrodeposited multilayers. – Co-Cu/Cu multilayers deposited from a simple sulfate bath were studied. By applying various Cu^{2+} concentration in the bath, the magnetic layers contained 45 to 99 at.% Co. The Cu layer thickness was varied between 0.37 nm and 3.45 nm. The magnetoresistance of these multilayeres exhibited the following features:

At each electrolyte concentration, the smallest copper layer thickness applied (0.37 nm) led to an anisotropic magnetoresistance (AMR) behaviour. At d(Cu) > 1 nm, the magnetoresistance curves showed GMR behaviour and the GMR value increased up to about d(Cu) = 2.6 nm. While samples deposited from dilute electrolytes with relatively high Cu layer thickness apparently saturated at about 2 kOe, the samples obtained from high Cu^{2+} concentration electrolytes could be saturated at fields higher than 8 kOe only.

The room-temperature magnetoresistance curves were decomposed into ferromagnetic (FM) and superparamagnetic (SPM) portions. The decomposition analysis revealed that the FM component of the magnetoresistance increased with d(Cu), and only a very little Cu^{2+} concentration dependence was obtained (Fig. 3.a). While the evolution of the FM part of the magnetoresistance with d(Cu) is fairly independent of the electrolyte composition, the SPM component of the magnetoresistance changed drastically with both d(Cu) and c(Cu^{2+}). At a particular electrolyte concentration, the SPM component first increased with d(Cu), passed through a maximum and then decreased (Fig. 3.b). The higher was the Cu^{2+} concentration in the electrolyte, the more significant SPM component was obtained. The decrease in GMR with d(Cu) above d(Cu) > 2.6 nm was due to the loss in the SPM contribution because the FM contribution kept increasing.

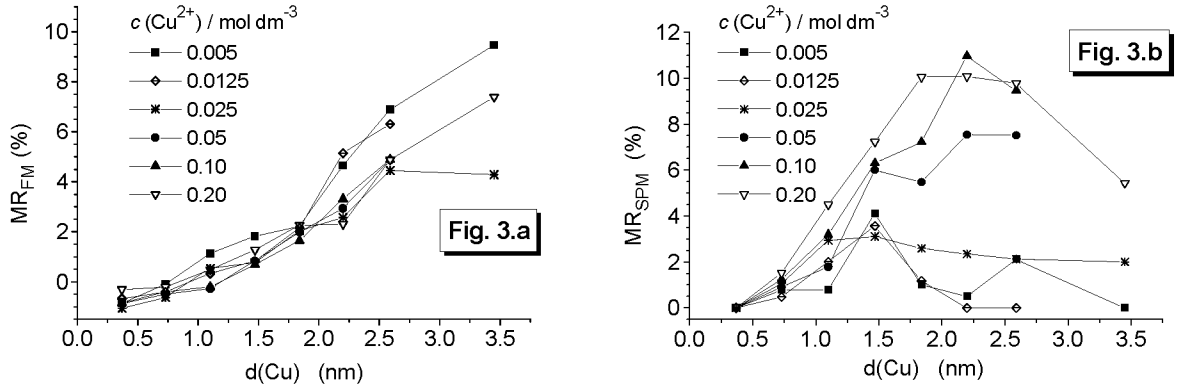

Figure 3. The FM component (a) and the SPM component (b) of the magnetoresistance of the Co-Cu/Cu multilayer samples

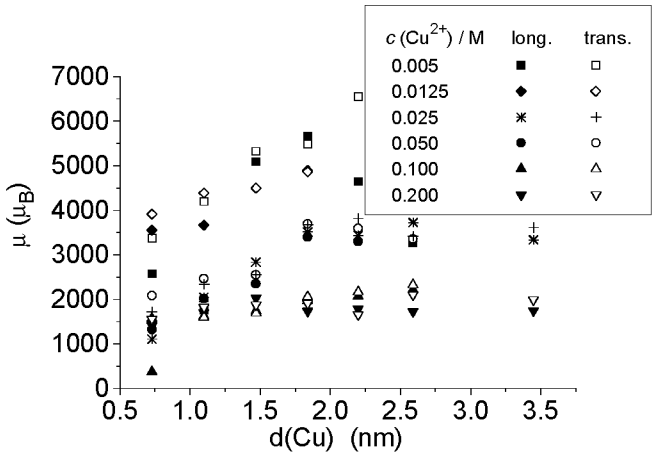

Figure 4.

The size of the SPM regions of the Co-Cu/Cu multilayer samples

The SPM-FM decomposition analysis also yielded the apparent size of the SPM regions (Figure 4). At d(Cu) > 2.5 nm, the SPM part of the magnetoresistance either vanished because the SPM grain sized tended to approach infinity ($c(Cu^{2+}) < 0.02$ moldm^{-3}) or saturated at a constant value.

The magnetoresistance properties observed were explained by the assumption that the magnetic layers were not homogeneous, and the constituents of the magnetic layers segregated already during the deposition process. The inclination of Co and Cu to segregate was further supported by their binary phase diagram that indicated mutual insolubility at room temperature under equilibrium conditions.

The result of the analysis led us to the conclusion that the SPM regions can be visualized as columnar objects ranging from the one copper layer to the neighbouring one.

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Grants and international cooperations

OTKA T 037673 Tunnelling magnetoresistance (TMR) in ferromagnetic/insulator nanostructures (I. Bakonyi, 2002-2005)

Wellcome Trust ISRF GR067595MA Study of partially structured protein solutions (Host: Institute of Enzimology of HAS, subcontractor participant: K. Tompa, 2005-2007)

Publications

Articles

H.1. Tompa K, Bánki P, Bokor M, Lasanda G, Varga LK, Champion* Y, Takács* L; Quadrupole effects in ^{63}Cu NMR spectroscopy of copper nanocrystals; *Appl Magn Reson*; **27**, 93-107, 2004

H.2. Bakonyi I; Atomic volumes and local structure of metallic glasses; *Acta Mater*; **53**, 2509-2520, 2005

H.3. Bakonyi I, Kiss LF, Varga* E, Varga LK; Magnetic properties of Ni-rich metastable Zr-Ni and Hf-Ni alloys; *Phys Rev B;* **71**, 014402/1-8, 2005

H.4. Bakonyi I, Péter L, Weihnacht* V, Tóth J, Kiss LF, Schneider* CM; Giant magnetoresistance (GMR) in electrodeposited multilayer films: the influence of superparamagnetic regions; *J Optoel Adv Mater;* 7, 589-598, 2005

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H.10. Kováč* J, Zentková* M, Bokor M, Mihalik* M, Kavečanský* V, Mitróová* Z, Zentko* A, Pekker Á, Kamarás K; Magnetic properties and ^{1}H NMR spectroscopy of $TM_2^{2+}[WIV(CN)_8]\cdot n H_2O$; *physica status solidi (c);* accepted for publication

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Materials, Processes and Devices (206th Electrochemical Society Meeting, Honolulu, Hawaii, U.S.A., 2004); Ed. S. Krongelb et al., The Electrochemical Society, Pennington, New Jersey, U.S.A., 2005; accepted for publication

See also: E.9., E.12., I.13., I.19.

I. METALLURGY AND MAGNETISM

L.K. Varga, I. Balogh, A. Bárdos[#], É. Fazakas[#], A. Kákay[#], P. Kamasa, G. Konczos, Gy. Kovács[+], J. Pádár, L. Pogány, F.I. Tóth, I. Varga

Soft magnetic nanocrystalline alloys. — A new family of cast-iron-based alloy compositions was developed which combines the good castability of the starting cast-iron alloy with the toughness conferred by Cr, Mo and Ga additions.

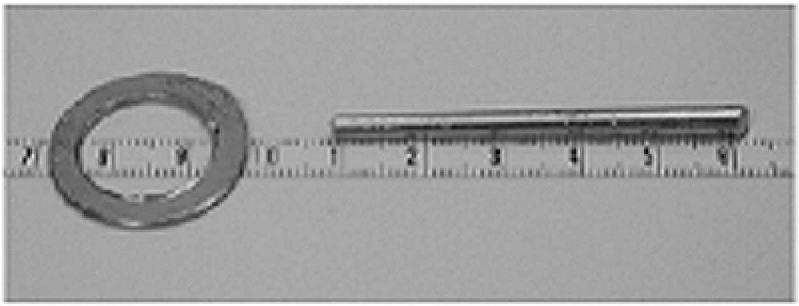

Figure 1. Photo of different shapes of cast bulk $Fe_{70.7}C_{6.7}P_{10.4}B_5Si_{1.1}Mn_{0.1}Cr_2Mo_2Ga_2$ amorphous alloy. Sample in ring shape has an outer diameter of 26 mm, an inner diameter of 18 mm and a thickness of 1 mm, and in rod shape a smaller diameter of 3 mm, a larger diameter of 4 mm and a length of 54 mm.

The new composition enabled us to obtain various forms of bulk amorphous material by net-shape-casting, such as rings and rods shown in Fig.1 having the largest sizes published so far in the literature. The excellent soft magnetic properties (H_c = 1.7 A/m and B_s = 0.5 T) obtained for the ring sample make it applicable for ring-core based sensors used for pressure measurements through the Villary effect.

A cheap cast iron based composition was developed ($Fe_{76}P_9C_8Si_2B_5$) containing no expensive glass former elements (Ga, Nb, Zr, etc.) which can be used for bulk amorphous powder production by gas atomization. Preparing 40 kg of powders in one cycle, we have demonstrated the possibility of scaling up the gas atomization process. The glassy powder was used for surface coating of various metallic materials by plasma spray. The coating regained its amorphous structure if special attention was paid for cooling the substrate material with a stream of air.

A new electrodeposition (ED) method was developed and patented to prepare nanocrystalline Fe sheets with flat hysteresis loops applicable up to 10 MHz. A plate transformer was prepared based on the ED nanocrystalline iron sheet using the usual integrated surface-mounted device (SMD) technology.

We have discovered a size dependence of the coercive field in the millimeter-centimeter range length scale of ribbon-like samples prepared from ultra soft amorphous and nanocrystalline alloys. This experimental result seems to be in contradiction with the general accepted size independence of coercivity for soft and hard magnetic materials. A model was proposed where surface pinned domain walls are considered with an effective stiffness constant linearly increasing with the demagnetization factor. We have got a formula for the coercive force, which is linearly dependent on the demagnetizing factor, N, for a given material and for a given shape:

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$$H_{c\,eff} = H_c + \frac{N}{8\mu_o} J_s S_V \cdot t$$

where, H_c is the coercivity of the initial long ribbon specimen, J_s is the saturation polarization, S_V is the area of the domain walls in a unit volume and t is the thickness of the ribbon. This size effect rules out the use of powder cores for high frequency power applications (f > 100 kHz and B ~ 0.2 T) because of the large hysteresis losses.

Micromagnetic modelling. — A new method has been developed to study the details of magnetic decoupling phenomena in two-phase nanocrytstalline alloys. The determination of the decoupling temperature for a two-phase nanocrystalline alloy has been so far based on the characteristic points in the evolution of the hysteresis loop parameters such as the coercive field and the B_r/B_s ratio versus temperature. However, these temperature dependences are not threshold-like but mostly smeared out in a rather wide range of temperature, making difficult to assess the right decoupling temperature. The decoupling phenomena in nanocrystalline alloys can be studied within the Preisach model, by recovering the Preisach map from the major hysteresis loops measured below and above the expected decoupling temperature. The Preisach map is defined by the function $\mu(h_1,h_2)$ where h_1 and h_2 are the switching up and switching down fields of the elementary Preisach operators. As the temperature increases the Preisach map (Fig. 2) is shifted from the region of reversible processes to the irreversible one and above a given temperature a two-peak feature appears in the irreversible region and the reversible part entirely disappears. Based on earlier calculations from the literature, this double-peak feature of the Preisach map can be interpreted by assuming a dipolar interaction between the monodomain particles. In this way the evolution of the temperature dependence of the Preisach map is able to assess the temperature where the coupling by exchange penetration is no more effective and the dipolar coupling remains the only interaction responsible for the hysteretic behavior of the

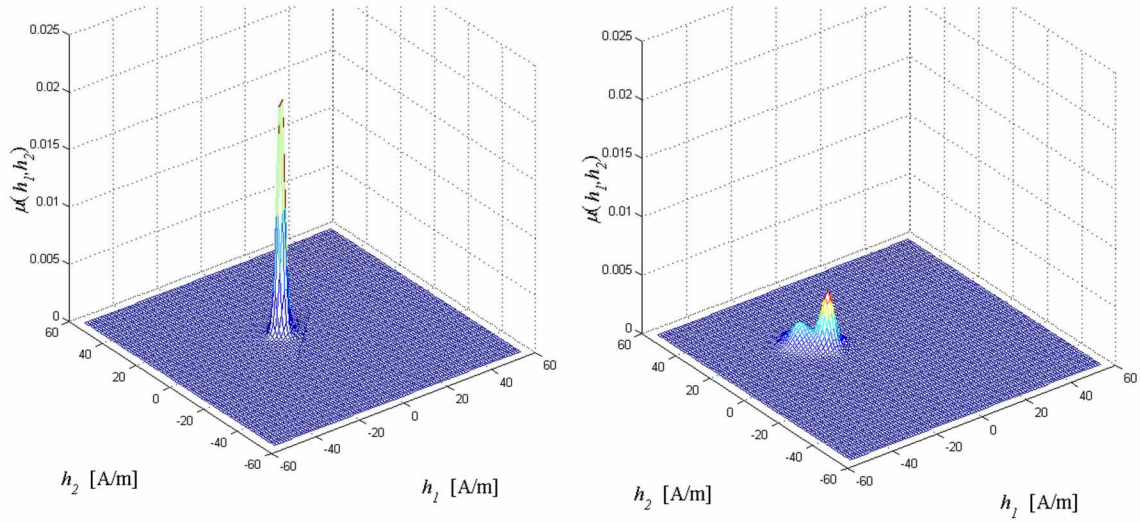

Figure 2. Preisach functions (maps) derived from the major hysteresis loops measured at 100 °C (left panel, below decoupling) and 460 °C (right pane, above decoupling)

interacting monodomain system.

Extracting domain wall patterns from SEM magnetic contrast images. — The magnetic contrast images of a soft magnetic metallic glass $Fe_{79}Si_6B_{14}Cu_1$ subjected to a periodic magnetic field were recorded with a scanning electron microscope by using a stroboscopic

technique. An image processing method for the extraction of domain patterns from these images was elaborated. Fig. 3a shows an intermediate state of the data processing.

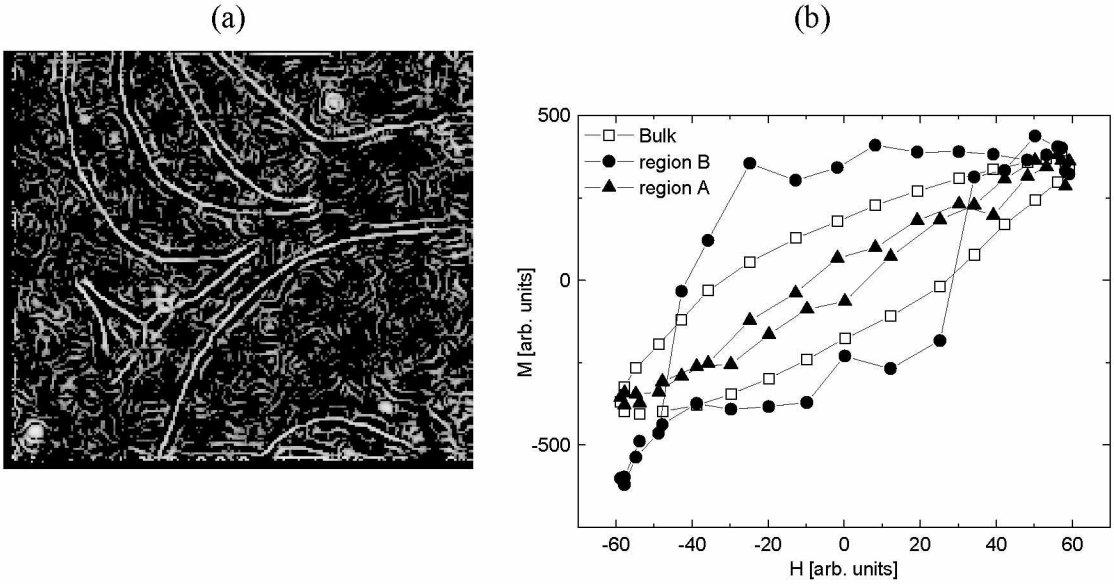

Figure 3. (a) Intermediate state of the image processing; (b) Comparison of local and bulk hysteresis loops

The information obtained in this way was used to reveal differences in the local magnetic behaviour of selected regions on the sample surface. Thus the effects of local fluctuations on domain behaviour have been made visible. In Fig. 3b, the calculated hysteresis loop of two regions of the sample surface is compared to the hysteresis loop measured over the whole sample volume (bulk).

Thermophysical properties of amorphous magnetic alloys. — An experimental setup for monitoring changes in physical properties such as thermal expansion, elasticity and magnetic induction for samples in the shape of thin ribbons was developed. A new sample holder for dilatometric measurement was designed to avoid buckling deformation for such ribbon materials. By simultaneously recording changes of different material properties, two observations were made in the temperature range below crystallization for amorphous $Fe_{85-x}Cr_xB_{15}$ alloys. First, there is a drastic change of the linear thermal expansion coefficient, α, upon the ferromagnetic–paramagnetic (FM–PM) transition. In the FM state, the coefficient α is approximately ten times lower than in PM state. This difference can be ascribed to the Invar effect where a lattice distortion due to spontaneous volume magnetostriction counteracts the normal lattice thermal expansion. A second effect related with sample deformation was observed just before crystallization. This effect is known as the softening of glassy materials when a glass-liquid transition takes place. Additionally, in the softening region a relaxation of the quenched-in enthalpy was observed in a DSC experiment. The work was supported by an exchange program between the Polish and Hungarian Academies of Sciences.

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Grants and international cooperations

OTKA T037643 Nanostructured functional coatings. Research grant for the Chemical Research Center of HAS (participant: L.K. Varga, 2002-2005)

NKFP-3A/0050/2002 Széchenyi NRP: Development of nanostructured coatings with unique properties by using environmental friendly methods (Participant: L.K. Varga, 2002-2005)

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HAS-SAS (Hungarian-Slovakian) Academy Exchange Programme: Study of physical properties of special magnetic materials (L.K. Varga, 2005-2007)

HAS-PAS (Hungarian-Polish) Academy Exchange Programme: Investigation of thermophysical properties of coatings (P. Kamasa, 2005-2007)

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See also: H.1., H.3., H.8.

J. NEUTRON SPECTROSCOPY IN CONDENSED MATTER

L. Rosta, L. Almásy, L. Cser, I. Füzesy, J. Füzi, Gy. Káli, A. Len[#], M. Markó[#], J. Orbán, E. Rétfalvi[#], Zs. Sánta[#], N.K. Székely[#], Gy. Török

The 10 MW Budapest Research Rector (BRR) and its experimental facilities on the KFKI site is a unique large-scale facility in the Central European region. The Neutron Spectroscopy Department is one of the Laboratories of the associate Institutes forming the Budapest Neutron Centre, which is open for the domestic and international user community and serves for basic and applied research, commercial utilisation and education. Experiments were completed in 2005 by the local staff and in collaboration with national or foreign users coming from university, industrial or other research laboratories. We operate several cold and thermal neutron beam instruments: a small angle scattering (SANS) spectrometer, a reflectometer (REFL), a three axis spectrometer (TASC) and a cold neutron beam test facility as well as a thermal beam three axis spectrometer (TAST) and time-of-flight diffractometer (TOFD). Our activity is based essentially on experiments performed on the above spectrometers, some special studies, however, were performed at other neutron source facilities e.g. at FZ Jülich, HMI Berlin, or LLB Saclay (France).

The scientific activity of our team is focused on neutron optics research, investigation of structure and dynamics of liquids, soft and solid matters as well as of materials with industrial relevance. A considerable effort of our team is also devoted to development of neutron scattering techniques.

Neutron holography. — The atomic resolution holography study of metal hydrogen systems was carried on. This activity was focused on the theoretical considerations of future aspects of the experiment. In order to broaden the materials to be investigated a single crystal NH_4Cl sample (size of $5x5x4mm^3$) was prepared. A large volume of methodical effort was successfully applied for furnishing a dedicated to neutron holography instrument, which is an optional use of the thermal 3-axis spectrometer.

Structure of ferrofluids. — Small-angle scattering of non-polarized neutrons was applied to reveal the character of the interparticle interaction in ferrofluids (FF). Scattering curves obtained at the SANS diffractometer of the Budapest Neutron Center were analyzed with respect to the scattering structure-factor reflecting this interaction. Two types of ferrofluids which are magnetite stabilized sterically in non-polar (benzene, cyclohexane) and polar (pentanol) carriers were studied. A significant difference between the two types of non-magnetized samples was observed. In the non-polar fluids the interaction effect on the scattering was small even for comparatively high volume fraction of magnetite (> 5 %), while in polar fluids it started to be visible above 1 %, which can be explained by the observed difference in the interaction potentials. The spatial correlations in FF with pentanol carrier have been also investigated as a function of concentration of the magnetic phase (c=0.6-20 % vol.) and temperature (20-85 C). We detected an anomalous increase of short range order by heating of low concentrated FF (c~0.6-4.0% vol.); the formation of short range order at ambient temperature was weakening at concentration growing c=7-14 % vol.; the structure was still stable at the highest concentration c~20 % vol. when particles' shell started to interpenetrate. The neutron scattering data reveal that the intrinsic magnetisation of particles is enhanced by the structural ordering induced.

Catalytic materials. — The atomic and cluster structure of Cu/ZnO based catalysts for methanol synthesis, reduced in hydrogen, has been studied by means of small–angle neutron

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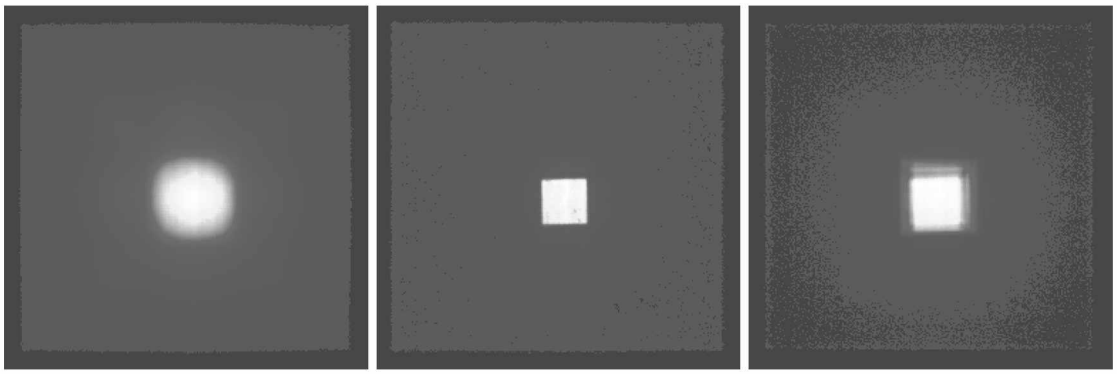
diffraction. The isotope substitution of Cu and H has been used for confirmation of the prediction on the mechanism that clusterisation takes place in the vicinity of Cu atoms. These inclusions at the surface of ZnO particles and inside of ZnO matrix have complicated structure: in the centre of a Cu cluster, which is surrounded by a hydrogen shell, the core is also formed of hydrogen. Such an arrangement of clusters apparently has a strong influence upon the catalytic activity of these compounds.

Instrumentation development. — A method for energy resolved neutron beam imaging has been developed based on position sensitive neutron detection in time of flight regime. It can be used for quality assessment of neutron optical elements (neutron guides, plugs, shutters, velocity selectors, focusing devices, monochromators), as a tool for verification of numerical simulation results for upstream components or it can provide input data for downstream optical element and instrument optimization (See Fig. 1).



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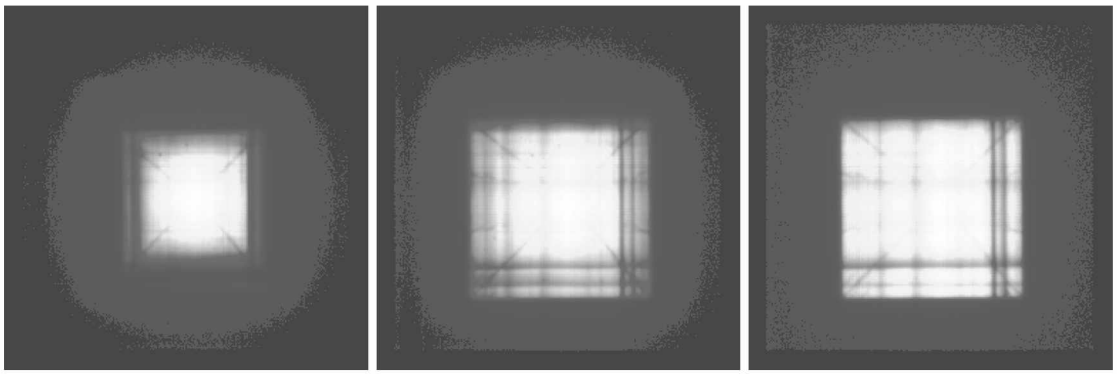

1.4 – 2.8 Å 2.8 – 5.6 Å 5.6 – 11.1 Å

Figure 1 Images of the LANSCE (spallation neutron source) FP12 beam in several wavelength ranges. The moderator is seen through the guide entrance right above Cd edge (0.5 Å). At higher wavelengths the whole guide exit (larger image due to perspective) is illuminated (the guide supermirrors come into effect).

Early 2005 a consortium of four institutes of the Hungarian Academy of Sciences lead by our Institute (as a member of the Budapest Neutron Centre) responded to the call for proposals (named Large International Projects, with Hungarian acronym NAP) by the National Office of Research and Technology. The proposal was selected for support in May and the project was started at September 1st for a 3 year period in 2005-08. It has 3 main objectives: a) improvement and development of equipment and access services at BNC; b) establish research and instrument development co-operation with Institute Laue-Langevin (ILL) at Grenoble, providing in this way formal access for the Hungarian R&D community to the world leading neutron facilities; c) perform high level research with special emphases

on bio- and nanotechnology related materials, engineering systems as well as for exploring objects of cultural heritage and ancient technologies. As a first step, an interim agreement was signed for the scientific membership of Hungary at the ILL. From January 2006 this agreement will be extended in a way that Hungary will join Austria and Czech Republic to form the CENI Consortium (Central European Neutron Initiative) for the ILL membership. Within the NAP project the instrument development programme will contribute to the construction of 2 new instruments at BNC (a polarised neutron reflectometer and a focusing SANS machine) as well as the new wide angle neutron spin echo spectrometer (WASP) at ILL.

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Grants and international cooperations

EU HII3-CT-2003-505925 Acces to Research Infrastructure (BNC, L. Rosta, 2004-2007)
EU HII3-CT-2003-505925 JRA2 Detector Development project (L. Rosta, 2004-2007)
EU HII3-CT-2003-505925 JRA3 Focusing Neutron Optics project (J. Füzi, 2004-2007)
EU HII3-CT-2003-505925 JRA2 Polarised Neutron Techniques (Gy.Török, 2004-2007)
OMFB-00478/2004 Atomic resolution neutron holography (L.Cser, 2004-2005)
NAP VENEUS-2005 OMFB-00648/2005 Visegrad Cooperation for Development and Application of Neutron Spectroscopy Techniques in Multidisciplinary Research (L. Rosta, 2005-2008)
CNRS-HAS 17212 Study of clustering and cooperativity in aqueous solutions of uncharged species by neutron scattering and computer simulations. (L. Almásy 2004 - 2005)
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TET RUS 13-2004 Nanoparticle (Gy. Török, 2005-2006)
TET RUS 14-2004 Neuholo (L. Cser, 2005-2006)

Publications

Articles

J.1. Balasoiu* M, Avdeev* MV, Kuklin* I, Aksenov* VL, Bica* D, Vékás* L, Hasegan* D, Török Gy, Rosta L, Garamus* VM, Kohlbrecher* J; Structural studies of ferrofluids by small-angle neutron scattering; *Magnetohydrodynamics*; **40**, 359-368, 2004

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K. NEUTRON SCATTERING

E. Sváb, M. Fábián[#], I. Harsányi[#], P. Jóvári, L. Kőszegi, Gy. Mészáros, L. Pusztai, L. Temleitner[#]

Amorphous materials and liquids. — Fine details of the microscopic structure of *amorphous silicon* have been investigated by comparing the structures of vapour deposited and ion-implanted samples. Via reverse Monte Carlo (RMC) analyses of the measured structure factors, it could be demonstrated that ion implantation leads to slightly less small bond angles than it was found for the evaporated material.

Since the early seventies several diffraction studies have been devoted to the structure of *amorphous Ge-Te*, especially $Ge_{15}Te_{85}$. Two models have been proposed on the basis of these experiments: in the 2-4 'textbook' model each Ge is coordinated by 4 Te atoms and each Te has 2 Ge or Te neighbours. The 3-3 model suggests that atoms are arranged in a basically 3-fold coordinated random network. To determine the coordination numbers and partial pair correlation functions we combined neutron- and X-ray diffraction data in the framework of a RMC simulation study. It has been shown that the Te-X coordination number (X=Ge, Te) is significantly higher than 2. On the other hand the Ge-Te coordination number varied between 3.4 and 4.0 in the several models tested. The combination of diffraction measurements with Ge-edge EXAFS data is in progress.

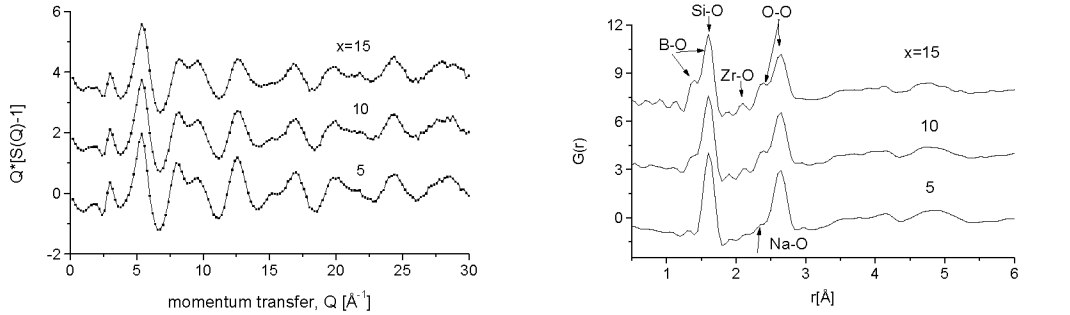

*Figure 1. Sodium borosilicate glasses (65-x)SiO_2*xB_2O_3*25Na_2O*5BaO*5ZrO_2 (x=5,10,15 mole%): a) neutron diffraction interference function b) reduced distribution function obtained by Fourier transformation. The curves are shifted vertically for clarity.*

Sodium borosilicate glasses are of significant current interest as suitable materials for isolating host media for radioactive waste material (i.e. U_2O_3 or PuO_2) storage. We have prepared multi-component sodium borosilicate glasses of the general composition (65-x)SiO_2*xB_2O_3*25Na_2O*5BaO*5ZrO_2 (x=5, 10, 15 mole%, where SiO_2 and B_2O_3 are strong network formers, Na_2O serves as network modifier; while BaO and ZrO_2 are glass and hydrolytic stabilizers. This matrix material has been doped by U_2O_3 (30wt%) or CeO_2 (10wt%), the latter models *PuO_2*. We have established that addition of U_2O_3 or CeO_2 does not cause any significant changes in the neutron diffraction total distribution function, meaning that the matrix glass serves as ideal recipient. This feature makes them suitable for radioactive waste material storage. To get a deeper insight into the atomic network configuration, we have measured the neutron diffraction pattern up to high momentum transfer values (Fig.1/a). The first neighbour distances were obtained from the total distribution functions (Fig. 1/b) due to the high r-space resolution. These values serve as constrains for RMC modelling to calculate the partial atomic correlation functions and

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coordination numbers. The detailed analysis of the first peak in the atomic pair correlation function reveals two different B-O nearest neighbour distances, which may be attributed to three and four coordinated borons. We suppose that the BO_3 groups form a vitreous v-B_2O_3 type network, while the negatively charged BO_4 groups are compensated by the cations and they form a v-SiO_2 type network.

Cu-based liquid metallic alloys are intensely studied due to their practical importance. We investigated liquid Cu-Sn alloys by modelling simultaneously X-ray and neutron diffraction measurements with the RMC technique. Due to the difference in the atomic sizes and scattering powers the three partial structure factors could be separated already on the basis of the two available measurements. Analysis of the resulting particle configurations has shown that the structure of these liquids is not homogeneous at the microscopic level. In the case of Cu_6Sn_5, for example, both the grouping of Sn atoms and the formation of Cu_3Sn-type associates can be observed.

The structure of *aqueous lithium-chloride solutions* has been studied via RMC modelling, at several electrolyte concentrations. Partial pair correlation functions were calculated directly from the particle configurations. Based on the O-H partial it may be suggested that at each electrolyte concentration, LiCl acts as a 'structure breaker' (Fig. 2/a): that is, increasing salt concentration causes an enhanced level of disruption of the hydrogen bonded network of water molecules. As far as the coordination of the cations is concerned (Fig. 2/b), it was established that up to the lowest concentration considered (LiCl:16H_2O), lithium ions have exactly 2 water neighbours up to a distance of 2.5 Å and another 4 to 5 neighbours up to 4 Å. At higher concentrations, the splitting of the hydration shell becomes less apparent. Concerning the hydration shell of the chloride ions (Fig. 2/c), a straight O-H…D hydrogen bond angle was found at each concentration. It was also found that not even at the highest concentration (LiCl:3H_2O) the smallest ion-ion distance is larger than the first ion-water distance (Fig. 2/d); that is, the existence of contact ion pairs may be excluded.

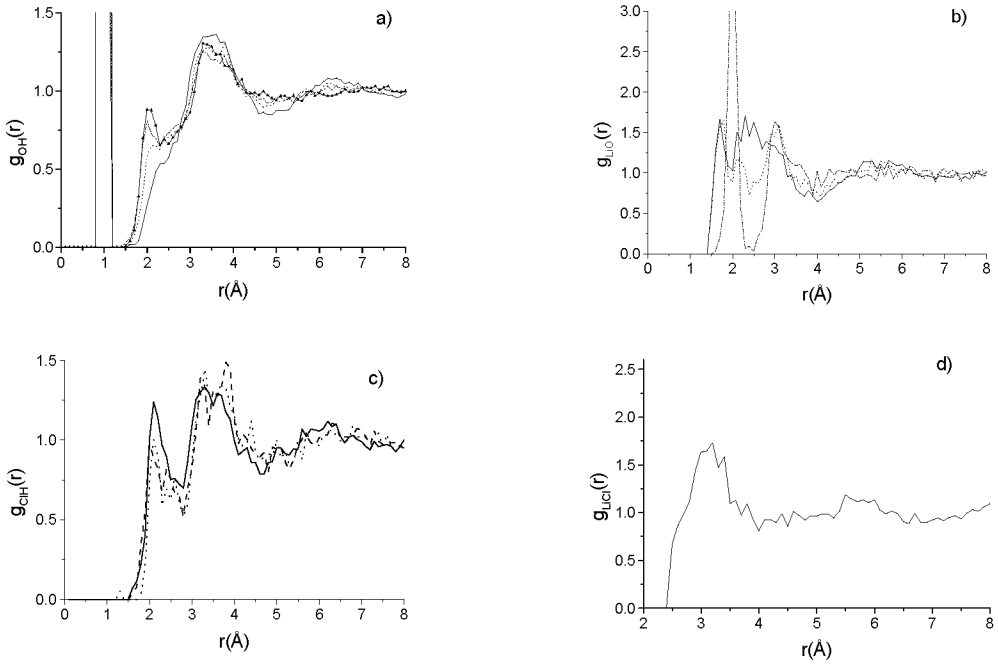

Figure 2. Partial pair correlation functions, $g_{ij}(r)$, calculated from the models for each concentration: LiCl.3H_2O (solid line), LiCl.8 H_2O (dotted line), LiCl.16 H_2O (dash-dotted line) and pure water (solid line with symbols). a): $g_{OH}(r)$; b): $g_{LiO}(r)$; c) $g_{ClH}(r)$; d) $g_{LiCl}(r)$.

Internal stresses. — We have investigated the texture of different *organ pipe brass tongue* by neutron diffraction using imaging plate technique. On the image 180° range of the diffraction cone was represented, which enabled to analyse the (111) and the (200) peaks of the brass reflections. Both ancient and new tongues were measured, and characteristic difference was recognised between these two groups. The new ones have typical rolling texture, whereas the old and hammered ones are more homogeneous namely they are almost isotropic.

Internal stress investigation by neutron diffraction was performed on $AlSi_{27}Ni_6$ sintered sample. Al(111), Si(220) and Al(200) peak shifts were measured to calculate the stresses inside the material. Similar composition of powder was used as reference material. Tensile stress was detected through the sample, which is more pronounced close to the surface of the rod.

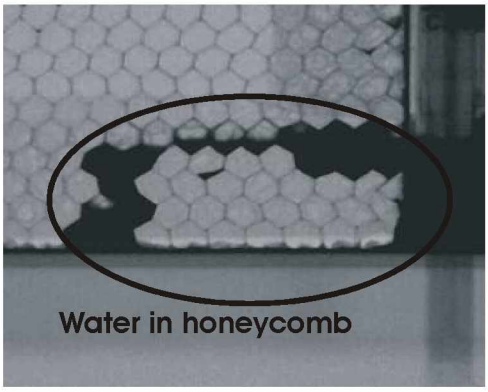

Figure 3. Water percolation in the honeycomb structure

Radiography. — In order to detect the possible defects in the composite structure of Mi-8 and Mi-24 type helicopter rotor blades used by the Hungarian Army, we have performed combined neutron- and X-ray radiography measurements. The most important points of our study have been the visualisation of the possible imperfections in the honeycomb structure, like: inhomogeneities of the resin materials at the core-honeycomb surfaces; defects at the adhesive filling; water percolation at the sealing interfaces of the honeycomb sections (Fig. 3); quality control of resin-rich mended areas; verification of the position of metal parts by X-ray; corrosion effects.

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Grants and international cooperations

OTKA T 042495 Neutron diffraction study of atomic and magnetic structures (E. Sváb, 2003-2006)

OTKA T 048580 Structural studies of liquids and amorphous materials by diffraction and computer modelling (L. Pusztai, 2005-2008)

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See also: D.7.

L. INTERACTIONS OF INTENSE LASER FIELDS WITH MATTER

Gy. Farkas, P. Dombi, S. Varró

Experimental research. – We analyzed sub-cycle dynamics of multi-photon-induced photoelectron emission from metal surfaces using a simple phenomenological model to assess optimum conditions for direct carrier-envelope phase measurement. To gain further insight femtosecond time-resolved measurements were carried out on a polycrystalline gold surface with pulses of a Ti:sapphire laser to explain the recently found, unexpectedly low carrier-envelope phase dependence of the photoemission process in this particular case. In the higher-order interferometric autocorrelation distribution, additional short side wings appeared suggesting that ultrafast dynamics of hot electrons reduce the carrier-envelope phase dependence of the photoemission electron yield produced by few-cycle laser pulses. Other metals can be investigated with this simple and fast method to pave the way towards the construction of a solid-state-based direct carrier-envelope phase detector.

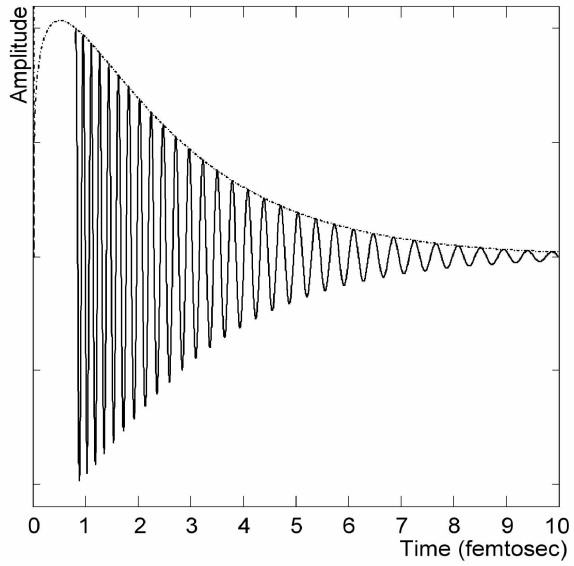

Figure 1. Precursor shape

We elaborated a new approach to generation of ultrashort (attosecond duration) pulses based on the Sommerfeld precursor phenomena. The numerical method for calculation of spectra of the first (Sommerfeld) precursor in a single-resonance Lorentz media based on representation of the initial signal as a sum of a number of semi-infinite pulses is developed for an arbitrarily shaped amplitude-modulated signal. Obtained spectra of the precursor generated by the signal created by "plasma mirror" technique show the potential possibility of production of electromagnetic pulses in attosecond regime (See Fig. 1.).

We also contributed to Ti:sapphire oscillator development efforts to push the limits of the energy of pulses directly coming from a Ti:sapphire oscillator. As a result, in the framework of a collaboration with the Max Planck Institute for Quantum Optics (Garching, Germany) pulse compression of so-called chirped-pulse oscillators was carried out together with pulse characterization.

Theoretical research. — On the basis of an exactly solvable model of classical electrodynamics we have determined the high-harmonic spectrum of a few-cycle Ti: sapphire laser radiation scattered on a plasma layer. The spectra obtained qualitatively differ from each other depending on the carrier-envelope phase difference of the incoming pulse. We have generalized the calculation to relativistic intensities, and, in addition, we have included the effect of a homogeneous external magnetic field. The spectrum of the magneto-Raman scattering can in principle be used to measure the mentioned absolute phase. Concerning quantum optics we have exatly determined the entanglement entropy of oscillator systems which were assumed to be in different sorts of many-particle radial wave packets. We have also described the detailed dynamics of the free evolution of such packets when the binding potential is suddenly switched-off.

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Grants and international cooperations

COST Action P 14 *"ULTRA"* Laser-matter physics with ultra-short pulses, high-frequency pulses and ultra-intense pulses. (Gy. Farkas, 2004-2008)

Hungarian State Eötvös Fellowship grant for P. Dombi at the Max Planck Institute for Quantum Optics, Garching, Germany (4 months)

OTKA T048324 Theoretical and experimental study of the newest nonlinear processes of 'attophysics' generated by superintense laser fields within the light wavelength and oscillation period scales (S. Varró, 2005-2007)

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See also: O.20.

M. LASER PHYSICS

K. Rózsa, G. Bánó, L. Csillag, Z. Donkó, P. Hartmann, P. Horváth[#], Z.Gy. Horváth, K. Kutasi, P. Mezei

Hollow cathode lasers. — Near 200 nm deep ultraviolet hollow-cathode metal ion lasers can be used as light sources for UV Raman and laser-induced fluorescent spectroscopy. These lasers are usually excited by charge transfer reactions between noble gas ions and metal atoms. High density of noble gas ions is created in hollow-cathode discharges while the necessary metal atom density can be produced either by thermal evaporation or utilizing the cathode sputtering effect of the discharge. High-voltage hollow-cathode arrangements have been developed during the last ten-year period to increase the efficiency of sputtered lasers. Our recent investigation is focused on the development of a 224 nm segmented hollow-cathode silver ion laser. Our aim is to prolong the lifetime of the laser tube in order to meet the requirements of commercial production. 150 mW peak power has been achieved using our latest model.

Gas discharge and plasma research. — We have experimentally investigated the electrical characteristics of steady-state low-pressure helium discharges. We have developed a two-dimensional hybrid model to study the spatial structure of a cylindrical helium discharge in a wide range of discharge parameters (electrode separation, pressure, voltage). We have carried out comparisons of one-, and two-dimensional models, and investigated the reliability of different (fluid-MC hybrid and Particle-in-Cell) discharge modeling techniques in general, for DC low-pressure discharges. In the field of strongly coupled plasmas we have studied the viscosity of two-dimensional Yukawa plasmas in their liquid phase. We have also investigated the structural (pair correlation function) and thermodynamic properties (correlation energy, compressibility), as well as the collective excitations through extensive molecular dynamics simulations of two-dimensional strongly-coupled Yukawa liquids. In cooperation with the HAS Research Institute for Particle and Nuclear Physics we have developed a quasi-classical model and molecular-dynamics simulation to investigate the properties of the strongly coupled quark-gluon plasma (sQGP) recently found in heavy-ion collision experiments.

Electrolyte cathode atmospheric pressure glow discharge (ELCAD). — A single capillary cathode construction of the ELCAD applying in a flow injection analysis system the subnanogram absolute limit of detection was received for heavy metals, but it was running with 3.5 ml/min sample flow wich is too high for capillary analytical systems. The another disadvantage of this arrangement is that the acidity of the basic electrolyte and the sample solution must be nearly the same (i.e. pH=1.55). To overcome these problems a new capillary ELCAD equipment was contructed wich operates with two solution streams within the cathode compartment. The concentric double capillary arrangement separates the basic electrolyte flow from the sample solution flow, thus the operation of the glow discharge itself becomes independent from the acidity of the sample solution. The detector dead volume is about 2 µl, the sample flow can be varied between 0.1-0.6 ml/min with water miscible composition (i.e. alcohols). The acidity of the plasma supporting electrolyte is pH=1.5 (HCl) and its flowing rate is 120 ml/h. The detector was tested by applying the flow injection of 0.2-1 µl of a multiple metal stock solution with 500 ng/µl concentration for each metals. Preliminary limit of detections: Cd 10 ng, Zn 30 ng, Cu and Pb 50 ng per elution peak. The response time is less than 1 s.

[#] Ph.D. student

Multispectral imaging reflectometer. — A new GVOP grant supports our R+D work in cooperation with the Research Institute for HAS Technical Physics and Materials Sciences. A pinhole based imaging system, with different (point and extended, multi-laser and multispectral incoherent) light sources enabled us to store and analyse incident angle and spectral dependent reflectivity data of the test surfaces. The obtained, polarisation, spectrum and angle dependent special images contain mostly all of the relevant data to analyse the surface properties of samples.

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Grants and international cooperations

OTKA T-48389 Modern plasma simulation techniques (Z. Donkó, 2005–2008)

MTA-OTKA-NSF 90/46140 Strongly coupled Coulomb systems (Z. Donkó, 2005-2007)

OTKA PD-049991 Post-doc position (P. Hartmann, 2005–2008)

OTKA T- 042493 The role of the ions of the basic electrolyte solution in the electrolyte cathode atmospheric glow discharge (P. Mezei, 2003–2006)

GVOP-3.1.1.-2004-05-0435/3.0 Multispectral imaging reflectometer (M.Fried and Z.Gy. Horváth, 2005-2007)

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M.17. Cserfalvi* T, Mezei P; Investigations on the element dependency of sputtering process in the electrolyte cathode atmospheric discharge; *Oral presentation on the European Winter Conference on the Plasma Spectrochemistry, 30 Jan-Febr 5, Budapest 2005* ,Compact disc, Ed: Fodor P.

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See also: O.20.

N. METAL OPTICS

N. Kroó, A. Hoffmann, Z. Lenkefi

Surface plasmon oscillations and their statistical properties. — Near field microscopy of plasmons generated in different layer structures was performed by means of a scanning tunneling microscope (STM). For the first time the signal fluctuations are statistically evaluated. The direct plasmon signal shows a narrow Gaussian or Poisson-like distribution whereas the thermal signal of the plasmon oscillation is described by a Boltzmann type distribution as it is expected for a signal of thermal origin. The fact that narrow Poissonian structures are observed indicates that the generated plasmon radiation may have non-classic properties which unfortunately cannot be proven unambiguously with our setup.

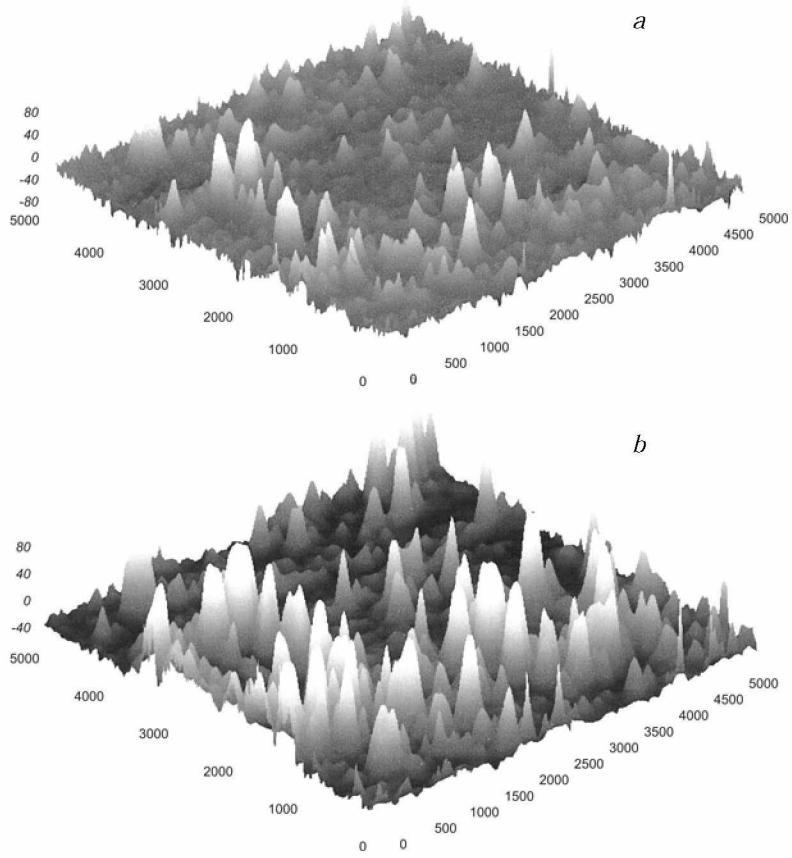

Figure 1. Surface plasmons created on a thin gold (mirror) layer, topography recorded in evanescent field (a) and a " thermal" map recorded simultaneously (b). The numbers in the X,Y,Z directions represent Å units.

For the excitation of surface plasmons (SPO) a 670 nm wavelength semiconductor laser has been used, chopped to get 50 μs long pulses with 1.8 kHz repetition frequency. The response of the STM to the illumination has been detected in two time windows of 15 μs duration. The first time window has been placed at the onset of the laser pulse, when only the SPO signal was expected (with minor thermal influence) and the second one 40 μs after the laser has been switched off when only thermal (thermoelectric and thermal dilatation) effects can be seen. These two types of pictures are shown in Fig. 1a and 1b.

In the experiments vacuum evaporated gold and silver surfaces with thickness between 30 and 50 nm were used. Images have been taken for sample areas between 0.2 x 0. 2 μm^2 and 10 x 10 μm^2.

The research work was carried out in strong cooperation with the STM group of the Max-Planck-Institute für Quantumoptik, München.

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International cooperations

Max Planck Institute for Quantum Optics (Garching, Germany): Surface plasmon research using STM (N. Kroó)

Physical Institute of University of Bonn (Germany): Charge density waves in photorefractive materials (Á. Hoffmann)

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O. LASER APPLICATION

A. Czitrovszky, M. Füle[#], P. Gál[#], H. Jancovius, P. Jani, Á. Kiss, M. Koós, S. Lakó, A. Nagy, D. Oszetzky[#], S. Tóth[#], L. Vámos[#], M. Veres[#]

Optical measuring techniques. — The instrumentation of our aerosol laboratory was improved with new devices. Among them an aerosol generating system for calibration of optical particle counters and sizers was developed. This system is based on a high resolution differential mobility analyzer supplied by GPR Vienna. The system can generate monodisperse aerosol particles from 5 nm up to 1 μm in diameter. Using this system the measuring head and electronic data evaluation system of a new dual wavelength forward-backward scattering laser particle spectrometer (DWOPS-1) were calibrated and tested. The system also makes the separation of certain aerosols to preset size ranges and investigation of their electric properties possible.

Atmospheric pollution. — A mobile laboratory for environmental monitoring of atmospheric pollution was enlarged and extended for new type of measurements. Chemical analysis of the aerosols collected by different samplers makes possible the determination of their composition. During 4 measurement campaigns the peculiarities of the atmospheric contamination were studied within the city of Budapest and its surrounding together with the experts of the National Public Health and Medical Officers Service. The mass- and number-concentration, size distribution, composition and spatial distribution of aerosols measured in different locations during different seasons of the year were determined. Complete databases containing all collected results were created. The measured parameters were compared with the statistics of the asthmatic and bronchial disease diagnosed in different seasons of the year.

In the frame of this project we developed also a simulation software package for the detection and determination of physical parameters of aerosol particles using the method of high frequency sampling techniques. In this simulation program the particle number was taken with Poissonian distribution, particle size with log-normal distribution. Using this software package we established that in a statistically constant ensemble the ratio of the mean value of scattered intensity to its standard deviation is the function of particle number only. It was proved that the time domain analysis of the scattered intensity can lead to the detection of other physical parameters, namely refractive index or particle composition. (The work was done in the frame of the National Research and Development Programme, Contract No. NKFP-3A/089)

Nanotechnology. — A high resolution interferometric surface testing system was extended for measurement of ragged surfaces by increasing the measuring range of the device. The measuring system was equipped by a new data evaluation system and software.

In the frame of this project a new improved algorithm was developed for the simultaneous measurement of velocity and size of nanometer size particles in photon correlation experiments. A theoretical detection limit for this type of size measurement method was established which now is around 50 nm. A new frequency stabilized semiconductor laser illumination device was constructed for the new photon correlator which is under construction. The measured frequency stability of this light source is around $\Delta f = 8.5\ 10^{-5}$ nm.

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Photon counting measurements of the statistical properties of different lights, generated by linear and non-linear sources, were studied. The statistics were compared with Poissonian statistic of coherent state. A quantum-optical measurement system for testing sensitive light detectors using non-classical light was elaborated.

The electronic and opto-mechanic units of a new type of light source with pre-determined photon number were elaborated. The laboratory setup for such new light source was constructed. (The work was done in the frame of the National Research and Development Programme, Contract No. NKFP-3A/071)

Amorphous carbon layers. — Photoluminescence emission - excitation spectroscopy combined with optical measurements was applied to characterise localized and quasilocalized electronic levels of amorphous carbon thin films. Tuning the photon energy used for excitation of light emitting optical transitions the composing bands of the broad photoluminescence spectrum were deconvoluted. Excitation spectrum of these composing bands was proven to have resonance feature. Taking into account the luminescence model of amorphous carbon films based on the radiative recombination of electron-hole pairs spatially localized in nanoclusters containing sp^2 hybridised carbon sites, we have determined exciton localization length and its distribution with peak energy of composing luminescence bands. The calculated values approach 1 nm, which corresponds to nanoclusters containing a few sp^2 carbon sites if they form linear chain arrangement.

The efficient light emission observable in a broad wavelength region from the photoexcited soft hydrogenated amorphous carbon thin films covers the ultraviolet- visible-near infrared region. This provides exellent potential for tuning working wavelength of optical devices. At the same time it is necessary to enhance narrow bandwidths from the inhomogeneously broadened spectrum. This can be achieved in a distributed Bragg reflector when microcavity structure is realised. Fabry-Perot resonance enhancement – inhibition of spontaneous light emission on self supporting a-C:H films have been observed. In Fig.1 this resonance effect appearing at different wavelengthes of the spontaneous emission band can be seen as a function of excitation energy for a-C:H film of 2099 nm layer thickness. The mode number of resonances were found between 11 and 17. The best quality factor of Fabry-Perot resonances measured was 40 and the line width was 15nm.

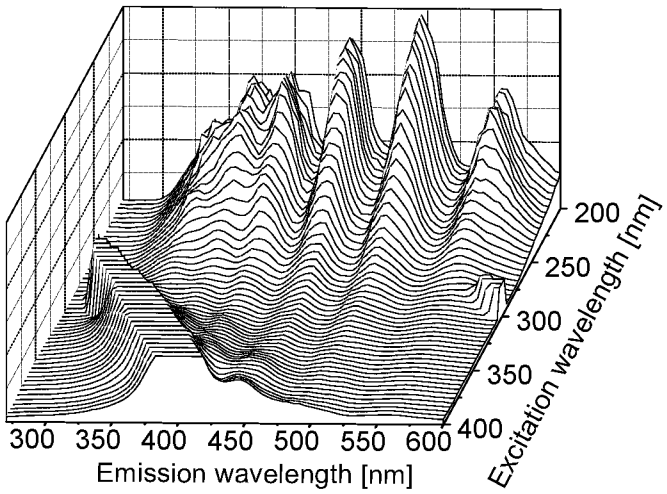

Figure 1. 3D excitation-emission PL spectrum measured on self-supporting a-C:H sample

Bio-, and haemocompatibility of carbon films opens an important application channel of amorphous carbon layers as protective coating on different medical implants. Our work focuses on the carbofilm covering of cardiovascular stents, which are made from stainless

steels of different compositions. As a first step the carbon films were deposited on plates of the different steels and the modification of their bonding properties with the composition of substrate material have been investigated by Raman spectroscopy. Adhesion force measurements by nanoindentation were also performed. The influence of surface treatement of metallic substrate by electrolitic polishing as well as by Ar^+ etching on the structure and adhesion of the covering carbon layer was also studied. We have concluded that carbon layers deposited with similar parameters exhibit graphitic character on Ni-rich Inconel alloys, while the covering layers are dimond-like films on Fe-rich stainless steels. Ar^+ etching enhances the adhesion of carbon films but electrochemical polishing was unfavoruable in this respect. (The work was done in the frame of the National Research and Development Programme, Contact No. NKFP-3A/042/04)

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Grants and international cooperations

NKFP-3A/089 National Research and Development Program, Environmental pollution of the atmosphere (A. Czitrovszky, 2004-2007)

NKFP- 3A/071 National Researh and Development Program, Nanotechnology II (Sub-coordinator: A. Czitrovszky, 2004-2007)

NKFP-3A/042/04 National Research and Developmment Program – Development of new generation coronary stents on the base of clinical experiences from haemocompatible materials coated by nanostrutured carbon (M. Koós, 2004-2006)

OTKA T-043359 Preparation and complex characterization of carbon based nano-composites (M. Koós)

NATO SfP-976913 Carbon Based Energy Storage (M. Koós, I. Pócsik, 2000-2005)

GVOP-3.1.1., No 0403/3.0, DIADEM (in cooperation with Budapest Technical University, coordinator: A. Czitrovszky, 2005-2007)

GVOP-3.1.1., No 0259/3.0 Photo-catalytic decomposition of pollutants (in cooperation with the University of Szeged, coordinator: A. Czitrovszky, 2005-2007)

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P. FEMTOSECOND LASERS

R. Szipőcs, Á. Bányász[#], J. Fekete[#]

Compact femtosecond pulsed lasers. — In collaboration with University of St. Andrews (Scotland), Sincrotrone Trieste S.C.p.A (Italy), MLD Technologies LLC (USA) and R&D Ultrafast Lasers Ltd (Hungary), we developed an improved version of ion-beam sputtered MCGTI mirrors with increased negative group delay dispersion (GDD) and red shifted reflection band aiming for applications in diode pumped, femtosecond pulse Cr:LiSAF lasers or in low pump threshold, 100-fs, tunable Ti:sapphire lasers. The computed group delay dispersion and reflectance of the mirror are shown in Fig. 1.

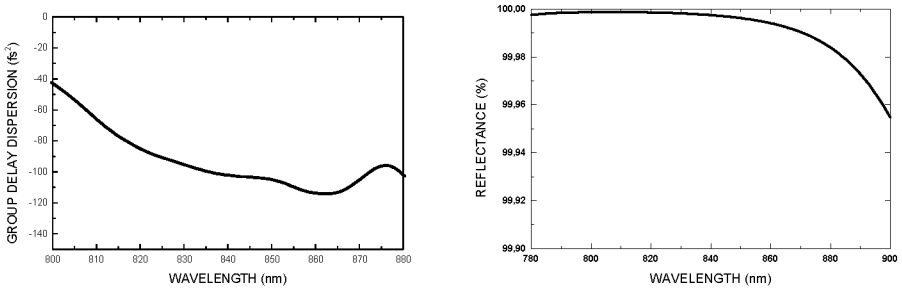

Fig. 1. Computed group delay dispersion and reflectance functions of the MCGTI mirrors developed for our femtosecond pulse, diode pumped Cr:LiSAF and low pump threshold, tunable Ti:sapphire oscillators

To demonstrate the performance of ion-beam sputtered multicavity Gires-Tournois interferometer (MCGTI) mirrors, we built Ti:sapphire and Cr:LiSAF laser oscillators pumped by compact laser sources with power as low as 1.2 W and 350 mW, respectively. In general, we used semiconductor saturable absorber mirror (SESAM) for mode-locking, but in some cases Kerr-lens mode-locking could be also used.

The dispersion of a highly doped, 4 mm long Ti:sapphire crystal was compensated by low reflection loss, negative dispersion MCGTI mirrors. These ion-beam sputtered mirrors were manufactured at MLD Technologies LLC, USA. The mirrors exhibite reflection $R > 99.97\%$ and negative GDD of -100 fs^2 in the 780-880 nm wavelength range. The relatively long Ti:sapphire crystal requires a high number of reflections on dispersive mirrors for proper dispersion-compensation (21 reflection in one roundtrip).

A relatively low pump power (1.2 W) at 532 nm still provided enough intracavity power for using hard aperture Kerr-lens mode-locking. Using Kerr lens mode-locking, output powers as high as 120 mW could be achieved with a $T = 5\%$ output coupler. In case of a $T = 2\%$ output coupler, we obtained mode-locked output powers of 40 mW and 85 fs pulse duration.

The MCGTI mirrors were also tested in a fs pulse Cr:LiSAF laser incorporating a SESAM pumped by a single, high-brightness diode laser with maximum output power of 350 mW at 670 nm wavelength. Modelocking started spontaneously at 10 mW of cw output power and up to 21 mW of mode-locked output power could be achieved.

Real time 3D nonlinear microscopy. — In collaboration with the Research Institute for Experimental Medicine, HAS (Budapest), we developed a novel two-photon microscope being capable of high speed measurement of neural networks or tiny neuronal structures

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such as spines in a 3D volume of approximately 0.6 x 0.6 x 0.2 mm^3, while keeping the advantages of a conventional two-photon microscope (e.g. high spatial resolution and high penetration depth). The basic idea that as follows: after taking a conventional 3D two-photon image of a biological sample, we determine the coordinates of those points (P_1, P_2 ...P_n) in the 3D volume that are to be investigated. During measurement of the neural activity, only these points are sequentially addressed by a high speed acousto-optic (AO) switch combined with a fiber boundle (comprising n pieces of single mode optical fibers) and a properly designed optical imaging system. The experimental setup for our proposed "real time 3D nonlinear microscope system" is shown in Fig. 2.

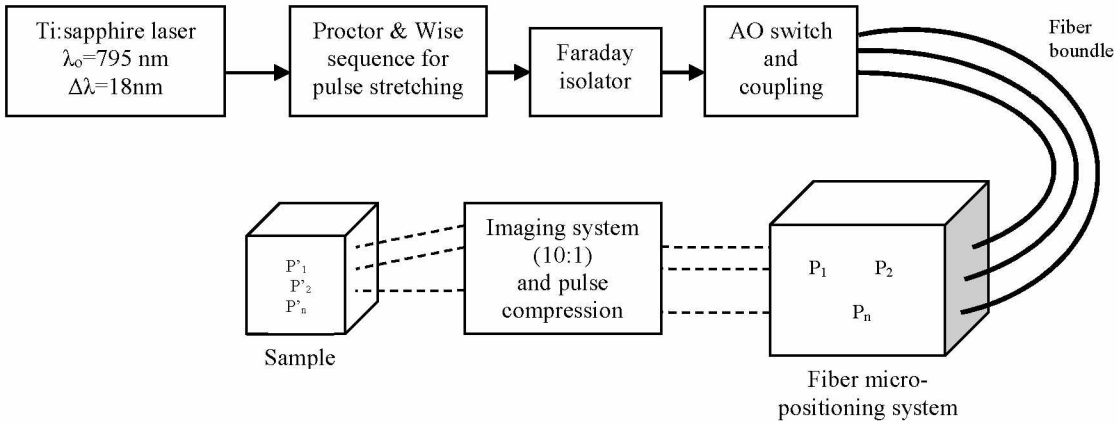

Fig. 2. Experimental setup for real time 3D two-photon imaging

Model-free deconvolution of ultrafast kinetic data. — Due to limitations imposed by the uncertainty relation between the spectral and the temporal pulse widths, selectivity in energy requires pulses used in femtosecond kinetic measurements whose widths are in the 100 fs range. As these pulse widths are comparable to characteristic times of the studied processes, this makes detection of the kinetic response functions inevitably distorted by convolution with the pulses applied. To restore the undistorted signal, deconvolution of the measured data is needed.

Our aim was to investigate the performance of the available methods capable of solving the convolution equation to get back the undistorted kinetic signal, without any presupposed kinetic or photophysical model of the underlying processes. In collaboration with the Department of Physical Chemistry of Eötvös University, Budapest thorough numerical tests of several model-free deconvolution methods were performed in order to select the most efficient methods. We have found that the model-free deconvolution gives satisfactory results compared to the classical "reconvolution" method where the knowledge of the kinetic and photophysical mechanism is necessary to perform the deconvolution. In addition, a model-free deconvolution followed by a statistical inference of the parameters of a model function gives less biased results for the relevant parameters of the model than a simple reconvolution. We have also analyzed real-life experimental data and found that the model-free deconvolution methods can be successfully used to get the undistorted kinetic curves in that case as well.

Singlet excited state behavior of pyrimidine bases in aqueous solution. — It was shown recently by several research groups that the singlet excited states of nucleic acid bases decay on the femtosecond timescale. One of us participated in steady-state and time-resolved spectroscopic study of uracil, thymine and 9 other derivatives of uracil (Francis Perrin

Laboratory, CEA Saclay). The excited state lifetimes were measured using femtosecond fluorescence upconversion technique in the ultraviolet. Experiments show that the excited state lifetimes of all the compounds examined are dominated by an ultrafast (<100 fs) component showing monoexponential decay. Only 5 substituted compounds show more complex behavior than uracil, exhibiting longer excited state lifetimes and biexponential fluorescence decays. A thorough analysis of the excited state potential energy surfaces, performed at the Time Dependent Density Functional Theory level in aqueous solution, shows that the energy barrier separating the local S1 minimum from the conical intersection increases going from uracil through thymine to 5-fluorouracil, in agreement with the ordering of the experimental excited state lifetime.

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Grants and international cooperations

OTKA T-049296 Propagation of ultrashort laser pulses in photonic crystal fibers and fiber amplifiers (R. Szipőcs, 2005-2007)

OTKA T-048725 Ultrafast linear and nonlinear processes in macromolecules (R. Szipőcs, 2005-2008)

NKFP 0394/2004 National Research and Development Program – New, low dispersion acousto- and electrooptic devices for femtosecond pulse lasers (Sub-coordinator: R.Szipőcs, 2005-2006)

NKFP 0182/2004 National Research and Development Program – Pump laser (Coordinator: R. Szipőcs, 2005)

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P.2. Bányász Á, Mátyus* E, Keszei* E; Deconvolution of ultrafast kinetic data with inverse filtering; *Rad Phys Chem*; **72,** 235-242, 2005

P.3. Bányász Á, Dancs* G, Keszei* E; Optimisation of digital noise filtering in the deconvolution of ultrafast kinetic data; *Rad Phys Chem*; **74,** 139-145, 2005

P.4. Gustavsson* T, Bányász Á, Lazzarotto* E, Markovitsi* D, Scalmani* G, Frisch* MJ, Barone* V, Improta* R; Singlet excited state behavior of uracil and thymine in aqueous solution: a combined experimental and computational study of 11 uracil derivatives; *J Am Chem Soc*; accepted for publication

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P.5. Várallyay* Z, Fekete J, Bányász Á, Szipőcs R; Sub-nanojoule pulse compression in small core area photonic crystal fibers below the zero dispersion wavelength; In:

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Q. OPTICAL THIN FILMS

K. Ferencz

Optical thin film structures consisting of nanoscale laminated layers. — We have continued our research concerning the development of optical thin film structures containing of nanooptically thick layers for advanced applications in laser physics and information technology. We have refined our new electron-beam deposition technology for producing of optical coatings containing nanooptically thick titania, silica, tantala, alumina, hafnia layers. Using needle-like optimization thin film design method, we have continued our research concerning the development of many kinds of ultrafast nanooptical coating systems – ultra-wide-band, low dispersion antireflection coatings, low dispersion beamsplitter coatings, ultrafast dichroic mirrors, wide-band output coupler mirrors, spectral shape filters for amplifiers, for example. Using the „OPTIMAC" optimization thin film design method, we have developed new type interference filter layer structures consisting of nanooptically thin metallic layers useful in the UV, VIS and IR spectral ranges.

Other developments on optical coatings. — Our work on ultrafast optical coatings is still in progress cooperating with the Max-Planck-Institute for Quantum Optics, Garching, Germany (Prof. Ferenc Krausz) for many types of advanced applications in laser oscillators, amplifiers, autocorrelators, coherent X-ray generation, etc. We have developed small-scale optical manufacturing technology for producing of large size fused silica compensating wedges having a few tenths of millimeter minimal thicknesses. We have arranged a new optical coating laboratory infrastructure financed by company Optilab Ltd. in our campus, where a new optical coating machine type INTEGRITY 36, manufactured by the US company DENTON VACUUM will start its operation in the near future. Our new coating machine manifests the state-of-the-art optical coating technology, the combination of ion-assisted deposition technology, oil-free cryopumping and a sophisticated computer control system.

We have continued the development of integrated optical grating couplers for biotechnological application as a switching or sensing element using bacteriorhodopsine as nonlinear optical material. Using our microstructured coating samples new types of biologically active nanotechnological devices are researched in cooperation with the Biophysics Institute at the Szeged Biological Research Centre of the HAS (Prof. Pál Ormos).

Based on our standard multiple-beam interference method for analysing optical coatings we have developed a new fast quantitative technique for analysing thin mineral oil films on water surfaces (project „Aquanal"). Using our CCD array spectrometer we have investigated the spreading phenomena of different kind of oil materials on water surfaces, and we have found that the equilibrium thickness of the oil films in many cases are much more larger than that of a monolayer. We plane to continue our research in this field using new type oil samples to understand the details of the interaction between mineral oils and water surface.

These results were obtained in the frame of the scientific cooperation between our Institute and Optilab Ltd., Budapest.

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Contract

OPTILAB-SZFKI No. 4056/2005

Grants and international cooperations

NATO SfP 974262 Optoelectronic Devices Based on the Protein Bacteriorhodopsin (Coordinator: C.E. Wolf, Germany, participant: K. Ferencz, 2000-2005)

NKFP3A/0005/2002 Nanobiotechnology: Elaborate a method to build nanotechnological devices for use in biology (Coordinator: P. Ormos, Szeged, participant: K. Ferencz, 2002-2007)

NKFP1A/0010/2002 Research and development of PET minicamera devices (Coordinator: L. Trón, Ped. Centre, Debrecen, participant: K. Ferencz, 2002-2007)

NKFP3A/071/2004 Nanotechnological material modifications and their metrology (Coordinator: J. Gyulai, MTA MFA, participant: K. Ferencz, 2004-2007)

NKFP3A/079/2004 On-site analysis of natural waters, geological media by micro- and nano-sensation methods („Aquanal") (Coordinator: I. Bársony, MTA MFA, participant: K. Ferencz, 2004-2007)

R. GROWTH AND CHARACTERIZATION OF OPTICAL CRYSTALS

I. Földvári, L. Bencs, E. Beregi, G. Dravecz[#], V. Horváth, Á. Péter, K. Polgár, Zs. Szaller

Growth and study of nonlinear borate crystals. — High resolution (0.04 cm^{-1}) absorption spectra of Dy in the self-frequency-doubling laser host, $YAl_3(BO_3)_4$ (YAB) single crystal were determined by Fourier Transform Spectroscopy in the (9-300 K) temperature range, and Dy^{3+} transitions from the $^6H_{15/2}$ ground state to the $^6H_{13/2}$, $^6H_{11/2}$, $^6H_{9/2}$+$^6F_{11/2}$, $^6H_{7/2}$+$^6F_{9/2}$, $^6H_{5/2}$, $^6F_{7/2}$, $^6F_{5/2}$, $^6F_{3/2}$, and $^4F_{9/2}$ excited states were identified and analyzed. The experimental energy levels were fitted with a single-ion Hamiltonian crystal-field model, and the crystal-field parameters were determined. The theoretically predicted quasi-quartet ground state was consistent with the experimentally observed 3.3 cm^{-1} first Stark splitting of the ground state of Dy^{3+}. The same fitting procedure was applied to analyze the previously published high resolution spectra of YAB:Er^{3+}, leading to a reliable unified picture for the two dopants. The exploited D_3 crystal field symmetry correctly described the experimental data giving an indirect confirmation that Er and Dy enter YAB by substituting Y in the trigonal prismatic sites. Moreover, the calculated energy levels outside the high-resolution energy limit used for fitting are in good agreement with independent standard resolution experimental data for both Er and Dy.

The two-photon-absorption coefficient (TPA) was determined for the nonlinear optical borates BBO (β-BaB_2O_4), LTB ($Li_2B_4O_7$) and CLBO ($CsLiB_6O_{10}$) grown in our laboratory. The intensity dependent (0.2-80 GW/cm^2) optical transition method was applied using 650 fs pulses of a KF excimer laser at 248 nm. For the measurements, only the homogeneous part of the beam (with a 4 mm circular aperture) was used and its far field image was focused into the samples, with a lens of 1 m focal length. Thus the beam distortion during measurement was negligible, except in the highest intensity range (around 80 Gw/cm^2) along the longest (15 mm) samples. The transmission curves were fitted by first principle model calculations. The determined TPA values for BBO (o-ray), BBO (e-ray), LTB and CLBO crystals are 0.5 cm/GW, 0.34 cm/GW, 0.22 cm/GW and 0.53 cm/GW, respectively.

Growth and study of stoichiometric $LiNbO_3$ single crystals. — MgO doped near-stoichiometric $LiNbO_3$ crystals have been grown by the high-temperature top-seeded solution growth method from the K_2O-Li_2O-Nb_2O_5 flux. The influence of the MgO doping on the liquidus surface was found to be minimal for low MgO concentrations (<2 mol %). Mg ions incorporate into the $LiNbO_3$ matrix with a segregation coefficient k>1, independently of the Li/Nb stoichiometry of the grown crystals. The typical concentration of MgO required for the growth of photorefractive damage (PRD) resistant (above threshold) crystals was shown reliant on the crystallization temperature. Therefore, by choosing an optimal combination of the crystallization temperature (i.e. Li / Nb ratio and K_2O content of the flux) and the amount of the dopant, the crystal properties can be tailored. In the Li_2O-Nb_2O_5-K_2O ternary system, the lowest value of the MgO dopant added to the melt where still above-threshold crystals can be grown was 0.2 mol%. At near-threshold MgO concentration, along the growth axis a transitional region was detected. The IR spectrum of this part of the crystal was characterized by the simultaneous presence of the two OH absorption bands (peaking at 3465 cm^{-1} and 3534 cm^{-1} frequency) corresponding to the below-threshold and above-threshold structures.

[#] Ph.D. student

The far-infrared (FIR) absorption coefficient and the index of refraction of undoped and MgO doped stoichiometric and congruent $LiNbO_3$ crystals were determined in the 30 – 180 cm^{-1} frequency range for polarization parallel to the Z axis, temperatures down to 10 K with different doping level of MgO. For stoichiometric $LiNbO_3$ smaller absorption and index of refraction were found, than for congruent samples. The FIR absorption coefficient has the lowest value in crystal with near-stoichiometric Li / Nb ratio and MgO content above the photorefractive threshold concentration. Therefore, in the terahertz range for efficient pulse generation the most suitable crystals are found to be of stoichiometric composition, doped with minimum amount of MgO required to reach the above-threshold level.

Two-color holographic recording was experienced in Tm-doped near-stoichometric $LiNbO_3$ single crystal. The UV-induced (355 nm) temporary absorption was followed with a 633 nm probe, and the rise time (2.6 s) and decay time (12 s) of it were determined. The UV-induced 0.2 cm^{-1} absorption coefficient change has led to 8% saturation diffraction efficiency in the gated four-wave mixing write process by 633 nm laser beams. Nonvolatile redout by 830 nm (3 W/cm^2) beam was demonstrated and explained by a three-center, two-color holographic recording process including small polarons. The overall performance of the $LiNbO_3$:Tm crystals in the gated nonvolatile holographic recording was better than that of the earlier results on $LiNbO_3$:Er.

Growth and study of paratellurite (TeO_2) and bismuth tellurite (Bi_2TeO_5) crystals. — Hybrid detectors (scintillating bolometers) are promising tools for rare event measurements like neutrino-less Double-Beta Decay (DBD). In such processes detectors of very low energy threshold and background are needed. TeO_2 is a unique combination of bolometer and source because the isotope ^{130}Te is DBD active, and because of the 33.87% natural abundance of ^{130}Te expensive enrichment procedure are not needed. Since the pure TeO_2 exhibits low luminescence output, the introducion of activator dopants was required. Successful growth of TeO_2 crystals with Mg, Mn, Nb and Zr dopants was first reported (10^{-4}-10^{-3} mol/mol in the melt). X-ray excited steady-state luminescence measurements revealed that Mn and Nb dopants are promising to enhance the scintillation light yield of TeO_2 crystals.
Bismuth tellurite, Bi_2TeO_5 is a prospective photorefractive material for multiplex holographic data storage. Due to its self fixing capability the recorded volume holograms do not require any further fixing between subsequent writes, or employing special recording schemes. Also, it accomplishes non-volatile readout of the holograms without additional system technology. The major shortcoming of Bi_2TeO_5 in holographic data storage is the long writing time required when using continuous wave (cw) laser beams. It was demonstrated that two-dimensional data pages could be recorded in bismuth tellurite crystals by nanosecond time scale pulsed laser (Nd:YAG, 532 nm, 3.5ns). Although the attained diffraction efficiencies were slightly below those observed in previous investigations using cw light, the photorefractive build-up time of the gratings is much shorter when using pulsed writing beams. The quality (bit-error-rate) and stability of the reconstructed digital data pages under permanent and pulsed read-out were also promising.

Application of analytical methods for optical crystals and other media. — Methods were studied and elaborated for the graphite furnace atomic absorption spectrometry (GFAAS) determination of Pd in environmental samples. The method included in the application of NiS fire-assay digestion and pre-concentration of Pd followed by its determination by GFAAS. The method was applied for the determination of Pd in roadside dust sampled from heavy traveled roads of Antwerp. This method is sensitive enough for the determination of ultra-trace levels of Pd and other platinum group elements in environmental samples.

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Grants and international cooperations

OTKA T-034176 Preparation and investigation of nonlinear optical crystals and crystal structures (K. Polgár, 2001-2005)

OTKA T-046481 Growth and spectroscopic investigation of self-frequency-doubling laser crystals (I. Földvári, 2004-2007)

OTKA T-046667 Materials and systems for high density data recording (E. Lőrincz, BME and I. Földvári, 2004-2006)

OTKA T038017 Development of laser ablation and electrothermal sample introduction methods for the atom spectrochemical study of element distributions (T. Kántor, ELTE, contributor L. Bencs, 2002-2005)

COST Action P8 Multinational EC program. Materials and systems for optical data storage and processing (H.-J. Eichler, Technische Universität, Berlin, Hungarian leader I. Földvári, 2002-2005)

HAS-Polish Academy bilateral cooperation program. Growth and spectroscopic investigation of rare-earth-doped nonlinear optical crystals (I. Földvári, 2005-2007). Partner: Institute of Low Temperature and Structure Research, PAS, Wroclaw

Hungarian - Italian Intergovernmental S & T Cooperation Programme. Growth and FTIR spectroscopy of optical crystals (L. Kovács, conributor I. Földvári, 2004-2007). Partner: Universita di Parma.

HAS - CNR Bilateral Cooperation Program. Growth and spectroscopic investigation of self-frequency-doubling laser crystals (I. Földvári, 2004-2006). Partner: Universita di Parma

EC-project No. EVK4-CT-2001-00067. Friendly Heating (R. Van Grieken, University of Antwerp, contributor L. Bencs)

HAS-Russian Academy Project 25. Investigation of crystal defects in broad forbidden band crystals (J. Janszky, contributor K. Polgár, 2005-2007). Partner: Joffe Phys. Techn. Institute, RAS, St.Petersburg.

HAS-Russian Academy of Sciences Project No. 26. Materials for solid state lasers and stimulated Raman emission (K. Polgár, 2005-2007). Partner: General Physics Institute, RAS, Moscow.

Bilateral (French-Hungarian) cooperation with University of Metz, MOPS, IUT St.-Avold, Common research on non-linear crystals and joint Ph.D. programs (K. Polgár and Á. Péter, 1999-open-end)

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Articles

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R.2. Péter Á, Polgár K, Ferriol* M, Pöppl* L, Földvári I, Cochez* M, Szaller Zs; Ternary system Li_2O-K_2O-Nb_2O_5 Part II.: Growth of stoichiometric lithium niobate; *J All Comp*; **368**, 246-252, 2005

R.3. Sosa* RF, Földvári I, Watterich A, Munoz* AF, Malliard* R, Kugel* G; Photoluminescence of Er^{3+} ions in Bi_2TeO_5 single crystals; *J Lumin;* **111**, 25-35, 2005

R.4. Földvári I, Beregi E, Capelletti* R, Baraldi* A; Visible range optical absorption of Er^{3+} ions in yttrium aluminum borate (YAB) crystals; p*hys stat sol (c);* **2,** 260-263, 2005

R.5. Álvarez* E, Sosa* R, Földvári I, Polgár K, Péter Á, Munoz AF*; Judd-Ofelt analysis and energy transfer mechanism in $LiNbO_3$: Er^{3+} single crystals; p*hys stat sol (c);* **2,** 175-179, 2005

R.6. Spolnik* Z, Bencs L, Worobiec* A, Kontozova* V, Van Grieken* R; Application of EDXRF and thin window EPMA for the investigation of the influence of hot air heating on the generation and deposition of particulate matter; *Microchim Acta;* **149**, 79-85, 2005

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R.16. Ravindra K*, Bencs L, Wauters E*, de Hoog J*, Deutsch F*, Roekens E*, Bleux N*, Berghmans P*, Van Grieken R*; Seasonal and site specific variation in vapour and aerosol phase polycyclic aromatic hydrocarbons over Flanders (Belgium) and their relation with anthropogenic activities; *Atmosph Environ;* accepted for publication

R.17. Divall* M, Osvay* K, Kurdi* G, Divall* EJ, Klebniczki* J, Bohus* J, Péter Á, Polgár K; Two-photon-absorption of frequency converter crystals at 248 nm; *Appl Phys B*; accepted for publication

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R.19. Pálfalvi* L, Hebling* J, Kuhl* J, Péter Á, Polgár K; Temperature and composition dependence of the absorption and refraction of Mg-doped congruent and stoichiometric $LiNbO_3$ in the THz range; In: *Proc. OSA Topical Meeting, 20th Anniversary Conference, Advanced Solid State Photonics, Vienna, Austria, 6-9 February 2005*; ISBN 1-55752-781-4; WB4, 2005

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R.21. Kontozova V*, Spolnik Z*, Worobiec A*, Godoi R*, Van Grieken R*, Deutsch F*, Bencs L; Assessment of air pollutant levels in some European museums and churches; In: *Cultural Heritage Conservation and Environmental Impact Assessment by Non-Destructive Testing and Micro-Analysis*; Eds.: René Van Grieken and Koen Janssens, Taylor and Francis Group, London; pp. 245-263, 2005

R.22. Bencs L, Ravindra* K, Van Grieken* R; Spatial and temporal variation of anthropogenic palladium in the environment; In: *Palladium Emissions in the Environment: Analytical Methods, Environmental Assessment and Health Effects*; Eds.: F. Zereini and F. Alt, Springer, Berlin; accepted for publication

R.23. Bencs L, Ravindra* K, Van Grieken* R, Determination of ultra-trace levels of palladium in environmental samples by graphite furnace atomic spectrometry techniques; In: *Palladium Emissions in the Environment: Analytical Methods,*

Environmental Assessment and Health Effects; Eds.: F. Zereini and F. Alt, Springer, Berlin; accepted for publication

Others

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See also: K.18., S.3, S.4. S.5

S. CHARACTERIZATION AND POINT DEFECT STUDIES OF OPTICAL CRYSTALS

L. Kovács, I. Bányász, G. Corradi, E. Hartmann, K. Lengyel[#], L. Malicskó, G. Mandula, A. Watterich

Microscopic studies on the early development stages of YAB crystals. — Small yttrium aluminium borate – $YAl_3(BO_3)_4$, YAB – single crystals spontaneously developed in ($K_2Mo_3O_{10}$ + B_2O_3) melt solutions were chemically extracted from solidified flux and studied by using optical and scanning electron microscopic methods. These small YAB crystals were found to be developed on small porous masses of microcrystallites which previously precipitated from the flux and whose compositions totally differed from that of YAB. This experimental result directly supports earlier assumptions on the nucleation of YAB and at the same time contributes to the explanation of certain grown-in imperfections observable within the YAB macrocrystals.

Investigation of point defects in $LiNbO_3$ single crystals. — Shallow Nb^{4+} and Ti^{3+} electron traps with d^1 type electon structure strongly influencing the holographic properties of $LiNbO_3$ and $LiNbO_3$:Mg have been characterised and compared by optical absorption and EPR spectroscopy, considering incorporation sites, electron-phonon interactions, and the possible associations as bipolarons.

Absorption bands of OH^- ions in $LiNbO_3$ crystals doped with Mg above the photorefractive threshold were investigated as a function of temperature up to 770 K. OH^- migration from the above-threshold environment to the below-threshold environment was observed with increasing temperature with a thermal activation energy of about 0.4±0.05 eV. For crystals at the Mg threshold it was shown that all hydroxyl ions can move to the intrinsic defects (Nb_{Li}-$4V_{Li}$) available in higher numbers than the OH^- ions. In the samples above but close to the threshold the amounts of intrinsic defects and OH^- ions are comparable, while in the samples far above the threshold there are no such intrinsic defects and the OH^- ions become "invisible" at elevated temperatures for the infrared absorption measurement.

A new interatomic potential which reproduces the structure and properties of the ferroelectric and paraelectric phases was used in calculations of the formation energies of intrinsic defects in $LiNbO_3$ crystals. Accordingly lithium Frenkel or Li_2O pseudo-Schottky disorder is expected to dominate and (Nb_{Li}-$4V_{Li}$) defect complexes are found to be energetically favourable in agreement with the experimental results.

Investigation of X-ray storage phosphors and scintillators. — The photo- and X-ray luminescence of Ce-doped fluorochlorozirconate glass-ceramics have been shown to have a number of different features compared to $BaCl_2$:Ce single crystals which are mainly due to the preferential incorporation of Ce into the glassy bulk instead of the orthorhombic $BaCl_2$ nanocrystal inclusions. The photostimulated luminescence (PSL), however, is still mostly related to Ce in the nanocrystal phase, which is consistent with the strongly reduced PSL intensity compared to single crystal samples. X-ray luminescence unrelated to Ce from the nanocrystal phase was also observed. On the other hand, the PSL efficiencies have been compared for $BaCl_2$:Ce, $BaBr_2$:Ce and BaFBr:Eu single crystals, the latter material being commercially used for the storage of X-ray images; $BaBr_2$:Ce was found to be at least comparable to BaFBr:Eu while $BaCl_2$:Ce is only slightly inferior as a storage phosphor.

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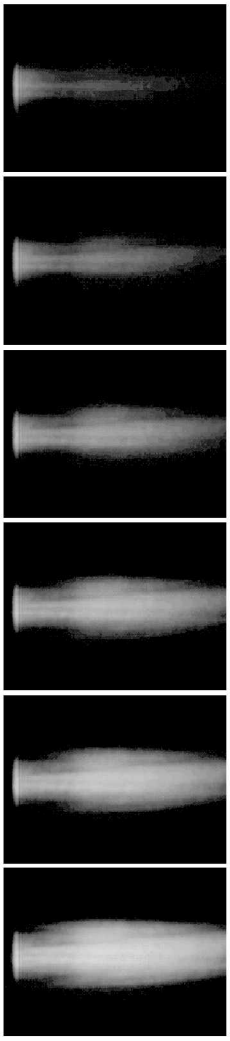

Spatial distribution, dynamics and neutron sensitivity of wave mixing holograms in $LiNbO_3$. — We showed experimentally for thick iron doped lithium niobate crystal, that the longitudinal distribution of a two-wave mixing refractive index grating is essentially the same during build-up and in the stationary state, with no change of its location either (Fig. 1.).

The decay, due to neutron irradiation, of a previously recorded photorefractive grating has been demonstrated experimentally in $LiNbO_3$:Fe single crystals. Calculations of the efficiency rate of the released nuclear energy invested to erase the grating by exciting electrons to the conduction band has given values between $(0.4 - 2) \times 10^{-3}$. A potential application of this phenomenon as a durable and erasable thermal neutron dosimeter suitable for repeated use has been proposed and the first experiments gave a sensitivity threshold of less than 0.4×10^{-10} cm^{-2} [the equivalent personal dose is $H_p(10,0^o) = 53$ mSv], which can still be decreased by optimizing doping level, oxidation state, OH^- concentration, and in addition, by ^6Li isotope enrichment. Additional studies on neutron activation of other elements than Li have also been carried out, in order to check the human radiation injury hazard during evaluation. We found that one day after the exposure the sample can be hazardous for human health only in case of a neutron fluence 3 order of magnitude higher than the maximal value measurable by the dosimeter ($\sim 10^{13}$ cm^{-2}).

Fig. 1. Dynamics of the build-up (photos in 15 s intervals) of a grating created by two-wave mixing. The recording beams are incident at the left hand side of the crystal. One can see that the peak builds up immediately in the middle.

Classical and digitally recorded holographic and diffractive optical elements and waveguides. — We improved our method for the determination of the temporal evolution of the profiles of photorefractive holographic gratings using both phase-contrast and interference microscopy. The range of the grating constants was extended down to 2 microns and up to 12 microns. The method for the determination of higher-order harmonics in phase holograms has been refined and checked using coupled-wave theory.

We succeeded in recording buried stripe waveguides in tellurite glass samples via implantation of high-energy N ions. The importance of this result lies in the fact that rare-earth element doped glasses – that are very promising candidates for active integrated optical elements – cannot be processed by standard microelectronic technology.

We realized high-resolution lensless Fourier-transform digital holography. This technique makes it possible to reduce the spatial frequency of the interference pattern to be recorded on the charge-coupled device (CCD), and consequently improves resolution of the reconstructed image. Holograms of micro lines of 8 μm width, recorded at $\lambda = 633$ nm, were successfully reconstructed. Nonlinearities of the recording device were taken into account at the numerical calculation of the holographic image.

History of Science. History of the Department. — The history of the departments for crystal physics and crystal technology started with the nomination of Z. Gyulai as full professor in 1935. The circumstances of the appointment were studied from the viewpoint of the decision-makers, the winner and the losers using archival sources. A film about Prof. Z. Gyulai and his coworkers in the fifties has been digitalized.

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Grants and international cooperations

OTKA T 034262 Investigation and optimization of crystalline and glassy systems for data processing (G. Corradi, 2001-2005)

OTKA T 035044 Gyulai-Tarján school in crystal physics (E. Hartmann, 2001-2005)

OTKA T 037669 Geometrical, vibrational and electronic structure of borate crystals and their defects (A. Watterich, 2002-2006)

OTKA T 047265 Photo- and neutronrefractive materials and phenomena (L. Kovács, 2004-2007)

TéT British-Hungarian Intergovernmental S & T Cooperation (GB-11/2003): Modelling of crystal defects in photorefractive materials (L. Kovács, 2003-2005)

TéT Austrian-Hungarian Intergovernmental S&T Cooperation (A-8/2003): Photorefractive materials and phenomena for lights and neutrons (L. Kovács, 2004-2005)

TéT Italian-Hungarian Intergovernmental S & T Cooperation (I-46/03): Growth and FTIR spectroscopy of optical crystals (L. Kovács, 2004-2007)

TéT Italian-Hungarian Intergovernmental S & T Cooperation (I-15/03): Fabrication of active and passive integrated optical elements and devices by ion beam implantation (I. Bányász, 2004-2007)

HAS – Polish Academy of Sciences joint project: Structure of real crystals (A. Watterich, 2005-2007)

HAS – Estonian Academy of Sciences joint project: Electronic paramagnetic resonance and time-resolved luminescence spectroscopy of oxyanionic crystals (A. Watterich, 2004-2006)

HAS – CNR joint project: Growth and spectroscopic investigation of self-frequency-doubling laser crystals (I. Földvári, contributor L. Kovács, 2004-2006)

HAS – Polish Academy of Sciences joint project: Growth and spectroscopic investigation of rare- earth-doped nonlinear optical crystals (I. Földvári, contributor L. Kovács, 2005-2007)

COST Action P8. Materials and Systems for Optical Data Storage and Processing (H.-J. Eichler, Berlin, Hungarian leader I. Földvári, contributor L. Kovács 2002-2005)

Long term visitors

— Margherita Mazzera, University of Parma, Italy, March-May 2005, 3 months (Host: L. Kovács)

Publications

Articles

S.1. Borowiec* MT, Watterich A, Zayarnyuk* T, Dyakonov* VP, Majchrowski* A, Zmiya* J, Baranski* M, Szymczak* H; Absorption and luminescence spectra of $KHo(WO_4)_2$ and $KEr(WO_4)_2$ single crystals (English translation of the Zhurnal Prikladnoj Spektroskopii **71**, 810-814, original in Russian); *Journal of Applied Spectroscopy*, **71**, 888-892, 2004

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S.3. Kovács L, Péter Á, Gospodinov* M, Capelletti* R; Hydroxyl ions in acousto-optic $Pb_5(GeO_4)(VO_4)_2$ and $Bi_2(MoO_4)_3$ single crystals; *phys stat sol (c)*; **2**, 689-692, 2005

S.4. Lengyel K, Péter Á, Polgár K, Kovács L, Corradi G; UV and IR absorption studies in $LiNbO_3$:Mg crystals below and above the photorefractive threshold; *phys stat sol (c)*; **2**, 171-174, 2005

S.5. Corradi G, Meyer* M, Polgár K; Bipolarons localised by Ti dopants in reduced $LiNbO_3$ crystals double-doped by Ti and Mg; *phys stat sol (c)*; **2**, 132-135, 2005

S.6. Selling* J, Schweizer* S, Spaeth* J-M, Corradi G, Edgar* A Williams* GVM; Radiation defects in Ce-doped $BaCl_2$ and fluorochlorozirconate glass-ceramics X-ray storage phosphors; *phys stat sol (c)*; **2**, 592-595, 2005

S.7. Bányász I; Refractive index modulation *vs.* before-bleach optical density modulation characteristics of silver halide phase holograms; *Optics Communications*; **244**, 79 -91, 2005

S.8. Mandula G, Rupp* RA, Balaskó* M, Kovács L; Decay of photorefractive gratings in $LiNbO_3$:Fe by neutron irradiation; *Applied Physics Letters*; **86**, 141107/1-3, 2005

S.9. Bányász I; Fourier analysis of high spatial frequency holographic phase gratings; *Journal of Modern Optics*; accepted for publication

S.10. Bányász I; Higher-order harmonics in bleached silver halide holograms; *special issue of Optics and Lasers in Engineering on Diffractive Optical Elements*; accepted for publication

S.11. Selling* J, Corradi G, Secu* M, Schweizer* S; Comparison of the luminescence properties of the x-ray storage phosphors $BaCl_2:Ce^{3+}$ and $BaBr_2:Ce^{3+}$; *J. Phys. Condens. Matter*; accepted for publication

Article in Hungarian

S.12. Hartmann E; Egyetemi tanári kinevezés 1935-ben (The appointment of professor Z. Gyulai in 1935, in Hungarian); *Fizikai Szemle*; **55**, 110-114, 2005

Conference proceedings

S.13. Righini* GC, Bányász I, Berneschi* S, Brenci* M, Chiasera* A, Cremona* M, Erht* D, Ferrari* M, Montereali* RM, Nunzi Conti* G, Pelli* S, Sebastiani* S, Tosello* C; Laser and ion implantation writing of integrated optical structures; In: *Photonic Materials, Devices and Applications, Sevilla, Spain, 9-11 May, 2005;* Ed.: G. Badenes et al.; Proceedings of SPIE; **5840**, 649 - 657, 2005

S.14. Bányász I, Kornis* J; High-resolution lensless Fourier-transform digital holography; In: *Optical Measurement Systems for Industrial Inspection IV, Munich, Germany, 13-16 June, 2005;* Ed.: W. Osten et al.; Proceedings of SPIE; **5856**, 71-79, 2005

S.15. Bugaychuk* S, Mandula G, Kovács L, Rupp* RA; Optical topographic technique to material characterization of photorefractive crystals; In: *The 10th International Conference on the Nonlinear Optics of Liquid and Photorefractive Crystals, Alushta, Crimea, Ukraine, 3-8 October, 2004;* Proceedings of SPIE; **6023**, 143-153, 2005

S.16. Mandula G, Rupp* RA, Balaskó* M; Erasure of elementary holograms in $LiNbO_3$:Fe by neutron irradiation; In: *International Conference on Holography, Optical Recording and Processing of Information, Varna, Bulgaria, 21-25 May, 2005;* Proceedings of SPIE; accepted for publication

S.17. Bányász I, Mandula G; Direct microscopic observation of hologram build-up in photorefractive crystals; In: *International Conference on Holography, Optical Recording and Processing of Information, Varna, Bulgaria, 21-25 May, 2005;* Proceedings of SPIE; accepted for publication

S.18. Selling* J, Corradi G, Secu* M, Schweizer* S; Rare earth doped barium halide x-ray storage phosphors and scintillators; In: *Proceedings of the International Conference on Inorganic Scintillators and their Industrial Applications (SCINT2005), Alushta, Crimea, Ukraine, 19-23 Sept. 2005*; accepted for publication

Others

S.19. Lengyel K, Kovács L, Péter Á, Polgár K, Corradi G, Baraldi* A; Temperature dependence of the OH absorption bands in $LiNbO_3$:Mg crystals at the photorefractive threshold; In: *Technical Digest of the International Workshop Lithium Niobate from material to device, from device to system, Metz, France, 23-25 May, 2005*; pp. 153-154

S.20. Jackson* RA, Lengyel K, Kovács L, Valerio* MEG; Computer modelling of the structure, properties and intrinsic defects in $LiNbO_3$; In: *Technical Digest of the International Workshop Lithium Niobate from material to device, from device to system, Metz, France, 23-25 May, 2005*; pp. 97-98

S.21. Corradi G, Meyer* M, Polgár K; Spectroscopy of shallow levels in $LiNbO_3$ systems and their role in material properties; In: *Technical Digest of the International Workshop Lithium Niobate from material to device, from device to system, Metz, France, 23-25 May, 2005*; pp. 117-118

See also: R.3, R.11, R.14.

T. NONLINEAR AND QUANTUM OPTICS

P. Ádám, J. Asbóth[#], P. Domokos, A. Gábris[#], J. Janszky, A. Kárpáti, Zs. Kis, T. Kiss, M. Koniorczyk, Z. Kurucz[#], V. Szalay, A. Vukics[#]

Laser-induced dynamics of atoms, cavity QED. — We generalized the optical dipole trap scheme by replacing the laser with a dynamical cavity field mode. For a large enough finesse, the far-detuned trapping field itself exerts a significant friction force so that stationary long-term trapping is obtained for arbitrary linearly polarizable particles. We have developed a fully quantum mechanical solution for this atom-cavity coupled system. Beyond the temperature and localization, the coherence properties of the atomic wave packet and its entanglement to the cavity field can also be calculated. This latter can be the source of a nonclassical photon statistics of the cavity field. Recently, we have been considering a field theoretical many-body description for the same system in the case of many atoms, which would allow us to study collective phenomena in the quantum mechanical regime of the system.

We have studied cavity QED systems composed of atoms externally trapped inside a cavity far detuned from the atomic transitions. We have found a scheme where even if the cavity interacts with the environment, universal quantum logic can be realized. The universality has been shown upto three qubits, but the formalism permits further generalization. Our further study to find more readily scalable schemes yielded a setup based on bi-modal cavities containing two modes of orthogonal polarizations with the same frequency, and four level atoms. Since during operation only the ground states are populated, another feature besides potential scalability is robustness against spontaneous decay.

We have shown that the STIRAP (stimulated Raman adiabatic passage) method can be extended to a nine-state system and the control of the polarization states of the pump and Stokes fields lead to a complete coverage of the five-dimensional final state space.

Quantum information, entanglement and teleportation. — We proposed the entanglement potential (EP) as a measure of nonclassicality for quantum states of a single-mode electromagnetic field. It is the amount of two-mode entanglement that can be generated from the field using linear optics, auxiliary classical states, and ideal photodetectors. The EP detects nonclassicality, has a direct physical interpretation, and can be computed efficiently.

We have derived the bound on the entanglement of three equally entangled orthonormal vectors spanning a three-dimensional subspace of the Hilbert space of two qubits, whose orthogonal complementary is a product state. We found that nonmaximally entangled measurements can optimize swapping of nonmaximal entanglement. We have related quantitatively the problems of generating cluster states with high values of concurrence of assistance, and of generating states with maximal bipartite entanglement in the system of many quantum bits. We have studied in detail the dynamical generation of such states with typical spin interactions in finite spin-1/2 systems.

We analysed the dynamics of single- and two-particle states in Ising-type passive quantum optical networks. The mutual entanglement was quantified using the concept of concurrence. We derived explicit expressions for the concurrence for single- and two-particle initial states in arbitrary passive networks and specified the result for Ising-type networks. We could show how to design a network in order to prepare a prescribed pattern of entanglement for

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one excitation. We found conditions to prepare the maximum attainable entanglement for passive optical networks in general.

We extended exact deterministic remote state preparation (RSP) to quantum systems of continuous variables. We proposed quantum optical protocols for continuous variable RSP of single-mode electromagnetic field states. We derived a general condition for that quantum information is transmitted securely in an exact deterministic RSP protocol.

Nuclear motion in molecules: dynamics and spectroscopy. — Two methods are developed, when solving the related time-independent Schrödinger equation, to cope with the singular terms of the vibrational kinetic energy operator of a triatomic molecule given in orthogonal internal coordinates.

It is shown, in the example of the water molecule, that state-of-the-art electronic and nuclear motion calculations, when allowance is made for their coupling, are capable of producing equilibrium structures for polyatomic systems somewhat more accurate than any of the experimental/empirical procedures.

The vibrational fundamentals and the rotational levels up to J=7 of two electronic states of CH_2 have been computed completely ab initio. The calculations were based on converged, variational nuclear motion calculations employing high-quality ab initio quartic force field approximations of the related potential energy surfaces.

A finite basis representation method has been developed for nondirect product basis functions of structure similar to that of spherical harmonics.

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Grants and international cooperations

OTKA T049234 Quantum optical systems and applications in quantum informatics (J. Janszky, 2005-2008)

OTKA T043079 Moving atoms and molecules in strongly-coupled radiation fields (P. Domokos, 2003-2006)

OTKA T043287 Adiabatic control in quantum optics and quantum informatics (Z. Kis, 2003-2006)

OTKA T045955 Theoretical methods to describe vibrational-rotational motion of molecules (V. Szalay)

TéT, Hungarian-Czech Bilateral Intergovernmental S&T Cooperation (CZ-5/03): Representing and processing quantum information in quantum optical systems (T. Kiss, 2004-2005)

TéT, Hungarian-Greek Bilateral Intergovernmental S&T Cooperation (GR-42/03): Nonlinear and quantum optics in photonic band gap materials: phenomena and methods (Z. Kis, 2005-2006)

FP6 Marie Curie European Reintegration Grant of the European Commission (MERG-CT-2004-502887), Collective dynamics of cold atoms in a cavity (P. Domokos, 2004-2005)

FP6 Marie Curie European Reintegration Grant of the European Commission (MERG-CT-2004-500783) Hawking radiation in the laboratory: quantum field theory in singular media (T. Kiss, 2004-2005)

Publications

Articles

T.1. Czakó* G, Furtenbacher* T, Császár* AG, Szalay V; Variational vibrational calculations using high-order anharmonic force fields; *Mol Phys*; **102**, 2411-2423, 2004

T.2. Giovanazzi* S, Farrell* C, Kiss T, Leonhardt* U; Conditions for one-dimensional supersonic flow of quantum gases; *Phys Rev A*; **70**, 063602/1-6, 2004

T.3. Zippilli* S, Asbóth J, Morigi* G, Ritsch* H; Forces and spatial ordering of driven atoms in a resonator in the regime of fluorescence suppression; *Appl Phys B: Lasers and Optics*; **79**, 969-978, 2004

T.4. Ádám P, Kárpáti A, Janszky J; Quantum trajectory method for determining the time evolution operator of dissipative quantum systems; *Acta Phys Hung B*; **23**, 35-40, 2005

T.5. Asbóth JK, Calsamiglia* J, Ritsch* H; A computable measure of nonclassicality for light; *Phys Rev Lett*; **94**, 173602/1-4, 2005

T.6. Czakó* G, Szalay V, Császár* AG, Furtenbacher* T; Treating singularities present in the Sutcliffe-Tennyson vibrational Hamiltonian in orthogonal internal coordinates; *J Chem Phys*; **122**, 24101/1-9, 2005

T.7. Császár* AG, Czakó* G, Furtenbacher* T, Tennyson* J, Szalay V, Shirin* SV, Zobov* NF, Polyansky* OL; On equilibrium structures of the water molecule; *J Chem Phys*; **122**, 214305/1-10, 2005

T.8. Gábris A, Agarwal* GS; Vacuum induced Stark shifts for quantum logic using a collective system in a high quality dispersive cavity; *Phys Rev A*; **71**, 052316/1-5 2005

T.9. Gábris A, Agarwal* GS; Controlled-NOT gates for four-level atoms in a bimodal cavity; *Acta Phys Hung B*; **23**, 19-24, 2005

T.10. Kárpáti A, Kis Z, Ádám P; Robust State Preparation in a Degenerate Four-State System; *Acta Phys Hung B*; **23**, 41-47, 2005

T.11. Kis Z, Vitanov* NV, Kárpáti A, Barthel* C, Bergmann* K; Creation of arbitrary coherent superposition states by stimulated Raman adiabatic passage; *Phys Rev A*; **72**, 033403/1-10, 2005

T.12. Koniorczyk M, Buzek* V; Nonmaximally entangled bases and their application in entanglement purification via swapping; *Phys Rev A*; **71**, 032331/1-10, 2005

T.13. Koniorczyk M, Rapcan* P, Buzek* V; Direct versus measurement-assisted bipartite entanglement in multiqubit systems and their dynamical generation in spin systems; *Phys Rev A*; **72**, 022321/1-12, 2005

T.14. Kurucz Z, Ádám P; Preparable ensembles for remote state preparation; *J Opt B: Quant Semiclass Opt*; **7**, 135-138, 2005

T.15. Kurucz Z, Ádám P, Janszky J; Simulating measurement statistics in remote state preparation; *Acta Phys Hung B*; **23**, 49-54, 2005

T.16. Novotny* J, Stefanak* M, Kiss T, Jex* I; Control of entanglement in Ising-type networks with one and two excitations; *J Phys A: Math Gen*; **38**, 9087-9103, 2005

T.17. Salzburger* T, Domokos P, Ritsch* H; Theory of a single-atom laser including light forces; *Phys Rev A*; **72**, 033805/1-10, 2005

T.18. Vukics A, Domokos P; Simultaneous cooling and trapping of atoms by a single cavity-field mode; *Phys Rev A*; **72**, 031401(R)/1-4, 2005

T.19. Vukics A, Janszky J, Domokos P; Cavity cooling of atoms: a quantum statistical treatment; *J Phys B: At Mol Opt Phys*; **38**, 1453-1470, 2005

T.20. Asbóth JK, Domokos P, Ritsch* H, Vukics A; Self-organization of atoms in a cavity field: Threshold, bistability, and scaling laws; *Phys Rev A*; **72**, 053417/1-12, 2005

T.21. Kurucz Z, Ádám P, Kis Z, Janszky J; Continuous variable remote state preparation; *Phys Rev A*; **72**, 052315/1-7, 2005

T.22. Czakó* G, Szalay V, Császár* AG; Finite basis representations with nondirect product basis functions having structure similar to that of spherical harmonics; *J Chem Phys;* accepted for publication

T.23. Furtenbacher* T, Czakó* G, Sutcliffe* BT, Császár* AG, Szalay V; The methylene saga continues: Stretching fundamentals an zero-point energy of $\tilde{X}^3B_1$ CH_2; *J Mol Struct*; accepted for publication

T.24. Koniorczyk M, Buzek* V, Ádám P; Simulation of generators of Markovian dynamics on programmable quantum networks; *Eur Phys J D*; accepted for publication

Article in Hungarian

T.25. Domokos P; Semleges atomok lézeres hűtése és csapdázása (Laser cooling and trapping of neutral atoms, in Hungarian); *Fiz Szemle*; **55**, 193–198, 2005

See also: S.26.

EDUCATION

Graduate and postgraduate courses, 2005

— Algebraic Bethe ansatz and its application (F. Woynarovich, ELTE[1])
— Advanced solid-state physics (J. Sólyom, ELTE)
— Renormalization methods for quantum systems (Ö. Legeza, ELTE)
— Statistical physics (F. Iglói , SZTE[2])
— Application of statistical physics (F. Iglói, SZTE)
— Disordered systems (F. Iglói, SZTE)
— Many body systems I. (P. Szépfalusy, ELTE)
— Many body systems II. (P. Szépfalusy, ELTE)
— The theory of magnetism I. (P. Fazekas, BME[3])
— The theory of magnetism II. (P. Fazekas, BME)
— Metal physics (J. Kollár, ELTE)
— Electronic states in solids (J. Kollár, ELTE)
— Advanced solid state physics II. (I. Tüttő, ELTE)
— Magnetic thin films (B. Újfalussy, BME)
— Solid state research I.-II. (I. Vincze, ELTE)
— Amorphous and crystalline materials (S. Kugler* and T. Kemény, BME)
— Macromolecules (S. Pekker, ELTE)
— Spectroscopy and material structure (K. Kamarás, BME)
— Infrared and Raman spectroscopy (K. Kamarás, BME)
— Physics of liquid crystals and polymers (Á. Buka and N. Éber, ELTE)
— Pattern formation in complex systems (Á. Buka, ELTE)
— Liquid crystals, their chemistry and chemical physics. (K. Fodor-Csorba)
— Non-conventional materials (Á. Buka, BME)
— Nanophase metals (I. Bakonyi, ELTE)
— Advanced material technology (G. Konczos, BME and ELTE)
— NMR spectroscopy (K. Tompa, BME)
— Group theory in solid state research (G. Kriza, BME)
— Superconductivity (G. Kriza, BME)

[1] ELTE = Loránd Eötvös University, Budapest
[2] SZTE = University of Szeged
[3] BME = Budapest University of Technology and Economics

— Application of thermal neutrons for study of condensed matter (L. Cser, ELTE).

— Introduction to neutron scattering (L. Cser, 3rd Regional Neutron Training Course, Budapest, 18-23 April, 2005)

— Mathematical modeling in electrical engineering (J. Füzi, TUBV[4])

— Computer aided design (J. Füzi, TUBV)

— Disorder in condensed phases (L. Pusztai, ELTE)

— Physics of amorphous matter I. (M. Koós, SZTE)

— Physics of amorphous matter II. (M. Koós, SZTE)

— From femtosecond lasers to attosecond physics (P. Dombi, SZTE)

— Optical signal processsing (R. Szipőcs, BME)

— Crystal physics of optical crystals (I. Földvári, Á. Péter, BME)

— Growth, processing and characterization of nonlinear optical crystals (In: Applied Lasertechnics, I. Földvári, BME)

— Theories of crystal growth (L. Malicskó, BME)

— Microscopy in materials science (L. Malicskó, BME)

— Technical application of crystals (E. Hartmann, BME)

— The characterization of crystals (E. Hartmann, BME)

— Electrodynamics (P. Ádám, PTE[5])

— Quantum mechanics I-II (P. Ádám, PTE)

— Theoretical physics (P. Ádám, PTE)

— Solid state physics (P. Ádám, PTE)

— Mechanics (J. Janszky, PTE)

— Quantum informatics (J. Janszky, PTE)

— Applied optics (T. Kiss, ELTE)

Laboratory practice and seminars

— Solid-state physics seminar (J. Sólyom, ELTE)

— Laboratory for solid state physics, Preparation and crystallization of metallic glasses (I. Vincze, ELTE)

— Lectures on vibrational spectroscopy (with laboratory practice), part of the course Experimental mMethods in materials science (K. Kamarás; BME)

— Infrared and Raman spectroscopy laboratory practice (K. Kamarás, BME)

— Infrared and Raman spectroscopy of carbon nanotubes; part of the Advanced molecular physics laboratory (K. Kamarás, ELTE)

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[4] TUBV = *Transilvania* University, Brasov, Romania

[5] PTE = University of Pécs

— Experiments on liquid crystals (Á. Buka and N. Éber, ELTE)

— NMR spectroscopy (K. Tompa, ELTE and BME)

— Physical chemistry laboratory practice (L. Péter, ELTE)

— Advanced solid state physics laboratory (Gy. Tóth, ELTE and BME)

— NMR (M. Bokor and G. Kriza, BME)

— Radiation protection laboratory practices (L. Temleitner, BME)

— Environmental protection laboratory practices: radiation aspects (L. Temleitner, BME)

— Medical application of lasers (Z. Gy. Horváth ; E-D Medical Laser Center)

— Vector calculus I, IV. (P. Ádám, PTE)

— Mathematical methods of physics (J. Asbóth, P. Ádám, PTE)

— Mathematical methods of physics I. (M. Koniorcyzk, P. Ádám, PTE)

Diploma works

— M. Karsai (SZTE): Nonequilibrium phase transitions in scale-free networks (Supervisor: F. Iglói)

— A. Szállás (SZTE): Renormalization of aperiodic quantum spin chains (Supervisor: F. Iglói)

— Á. Pekker (BME): Wide-range optical spectroscopy of carbon nanotubes (Supervisor: K. Kamarás)

— B. Császár (BME): Dioda pumped, femtosecond pulse Cr:LISAF laser (Supervisor: R. Szipőcs)

— J. Fekete (ELTE): Modelling and measurement of a fiber delivery system for a two-photon absorption fluorescence microscope (Supervisor: R. Szipőcs)

— T. Furtenbacher (ELTE): Variational calculation of the rotational-vibrational spectra of triatomic molecules; (Supervisor: V. Szalay and A.G. Császár)

— Á. Nagy (ELTE): Calculation of vibrationally averaged molecular constants for small molecules, and application of temperature-dependent basis functions to model systems; (Supervisor: V. Szalay and A.G. Császár)

Ph. D. students

K. Buchta (ELTE): Phase transitions in low-dimensional spin and fermionic models (Supervisor: J. Sólyom)

E. Szirmai (ELTE): Mott-transition in SU(n) symmetric Hubbard chains and ladders (Supervisor: J. Sólyom)

F. Bagaméry (SZTE): Critical behaviour of 2d models with inhomogeneous perturbations (Supervisor: F. Iglói)

L Környei (SZTE): Statics and dynamics of random-field Ising models (Supervisor: F.Iglói)

P. Nagy (SZTE): Relaxation in complex networks (Supervisor: F. Iglói)

F. Borondics (ELTE Graduate Program in Chemistry, supported by HAS): Raman spectroscopy of carbon nanotubes (Supervisor: K. Kamarás)

Gy. Pergerné-Klupp (ELTE Graduate Program in Chemistry, supported by HAS): Jahn-Teller distortions in alkali fulleride salts (Supervisor: K. Kamarás)

Á. Pekker (BME): Spectroscopy of chemically functionalized carbon nanotubes (Supervisor: K. Kamarás)

É. Kováts (ELTE): Addition reaction of fullerenes and related compounds in solid phase (Supervisor: S. Pekker)

G. Tóth (ELTE): Field theoretic description of far-from-equilibrium solidification morphologies (Supervisor : L. Gránásy)

A. Bárdos (BME): Preparation, characterization and application of Fe-based bulk amorphous alloys (Co-supervisor: L.K. Varga)

É. Fazakas (ELTE): Preparation of bulk amorphous alloys by mechanical alloying (Supervisor: L.K. Varga)

A. Kákay (ELTE): Magnetic nanocomposites: modelling and experiments (Supervisor: L.K. Varga)

L. Németh (BME): NMR study of low-dimensional metals (Supervisor: G. Kriza)

P. Matus (BME): NMR study of metals with correlated electronic system (Supervisor: G. Kriza)

Á. Pallinger (ELTE): Dissipation in Type-II superconductors (Supervisor: B. Sas)

I. Varga (BME): Magnetic domain contrast studies and image processing by SEM (Supervisor: L. Pogány)

M. Markó(BME): Neutron holography (Supervisor: L. Cser)

L. Temleitner (BME): Diffraction and computer simulation studies of disordered molecular systems (Supervisor: L. Pusztai)

I. Harsányi (ELTE): The structure of aqueous electrolyte solutions (Supervisor: L. Pusztai)

M. Fábián (ELTE): The structure of borosilicate glasses (Supervisor: E. Sváb)

P. Horváth (ELTE): Mass spectroscopic studies of radiofrequency H_2 and SiH_4-H_2 plasmas (Supervisor: K. Rózsa)

S. Tóth (SZTE): Light emission of carbon based films and nanoclusters (Supervisor: M. Koós)

M. Füle (SZTE): Optical absorption investigation of hydrogenated amorphous carbon films (Supervisor: M. Koós)

P. Gál (BME): Development of light scattering instruments (Supervisor: A. Czitrovszky)

D. Oszetzky (BME): Application of quantum-optical measurement methods (Supervisor: A. Czitrovszky)

L. Vámos (BME): Statistics of scattered light (Supervisor: P. Jani)

G. Dravecz (ELTE and Université de Metz): Study of the phase equilibria and crystal growth in the ternary system A_2O-Li_2O-M_2O_5 (A= K,Rb,Cs, M=Nb,Ta) (Supervisor: K. Polgár)

A. Bahouka (Université de Metz): Comparative study of the physical properties of borate single crystals prepared by different methods (Hungarian supervisor: K. Polgár)

A. Gábris (SZTE): Nonlinear photonic crystals and quantum optical processes therein (Supervisor: J. Janszky)

Z. Kurucz (SZTE): Quantum state manipulation and quantum information theory (Supervisor: J. Janszky)

A. Vukics (SZTE): Dissipative motion of atoms in strongly-coupled light fields (Supervisor: P. Domokos)

J. Asbóth (SZTE): Atom-atom interactions mediated by optical resonator fields (Supervisor: P. Domokos)

Dissertations

Z. Donkó: Computer modling of low-pressure gas discharges and strongly-coupled plasmas (D.Sc., Hungarian Academy of Sciences)

Zs. Gercsi: Tayloring the hysteresis loop for high frequency and high temperature applications of nanocrystalline alloys (Ph.D., ELTE – ENS de Cachan, France; Hungarian co-supervisor: L.K. Varga)

Shapaan Mahmoud Shapaan: Thermal stability and glass-forming ability of iron and cast iron based bulk amorphous alloys. (Ph.D., ELTE, co-supervisor: L.K. Varga)

L. Kőszegi: Induced and as-quenched stresses in magnetic amorphous alloys (Ph.D., ELTE)

M. Veres: Raman scattering of amorphous carbons (Ph.D, BME, supervisor: M. Koós)

K. Lengyel: Investigation of the absorption of OH vibrations in oxide crystals (Ph.D., SZTE, supervisor: L. Kovács)

G. Mandula: Novel methods and applications of spatial and temporal investigation of wave-mixing in photorefractive crystals (Ph.D., BME, supervisor: L. Kovács)

AWARDS

— N. Kroó, Honorary Medal „De Scientia et Humanitate Optime Meritus" awarded by the Academy of Sciences of the Czech Republic

— N. Menyhárd, Main Physics Award of the Hungarian Academy of Sciences

— F. Iglói, Physics Award of the Hungarian Academy of Sciences

— L. Gránásy, Physics Award of the Hungarian Academy of Sciences

— L. Vitos, Bolyai-Plaquette 2004, Hungarian Academy of Sciences

— L. Gránásy, T. Pusztai, T. Börzsönyi, G. Tegze, Trophy Award of the Mater. Res. Soc.

— L.K. Varga, SZFKI Annual Publication Award (2005)

— G. Bortel, Bolyai Grant (2003-2006)

— G. Oszlányi, Bolyai Grant (2003-2006)

— T. Pusztai, Bolyai Grant (2003-2006)

— T. Börzsönyi, Bolyai Grant (2005-2008)

— L. Péter, Bolyai Grant (2004-2006)

— R. Szipőcs, Bolyai Grant (2004-2005)

— P. Domokos, Bolyai Grant (2003-2006)

— J. Fekete: OTDK National Conference of Student Research, Optics 1. prize

CONFERENCES

— Workshop **Quantum Mechanical Studies of Solid Surfaces**, Budapest, June 30-July 2, 2005. Organizers: János Kollár, Krisztina Kádas, Levente Vitos. The purpose of the meeting was to provide an overview on the participants' recent activity about studying the surface properties of metals and alloys, and stimulate cooperation in these fields. 20 participants have attended the workshop.

— The **Third Central European Training School on Neutron Scattering and COST Training School on Neutron Optics (CETS2005)** organized by the Neutron Spectroscopy Department was held in Budapest from April 18-23, 2005. The scope of this course was to provide insight into neutron scattering techniques and their application for studies on structure and dynamics of condensed matter. This training opportunity was offered to the European community with special emphasis on the Central European region and with a special regard on neutron optics. The 18 hours of lectures given by scientists from the leading European neutron centers (ILL-Grenoble, HMI-Berlin, LLB-Saclay, JINR-Dubna, NPI-Prague, BNC-Budapest, University of Vienna) gave an introduction on neutron scattering techniques; the experiments on neutron spectrometers have demonstrated to the students the art of utilization of instruments at a large scale facility. Experiments on the following equipment were performed: small-angle neutron scattering instrument, three-axis spectrometer, neutron reflectometer (multilayer reflectivity), prompt-gamma activation analysis, data imaging and analysis of anisotropic scattering spectra, and neutron focusing with magnetic lenses (hexapole magnets). The school provided a forum for the presentation and discussion of actual research works of young scientists in the course of a half-day program, which was devoted to a poster/short oral presentation session. The participants (33 students) were young physicists, chemists, biologists, and actual or potential neutron users from the different countries of Europe (Austria, Bulgaria, Czech Republic, France, Hungary, Italy, Portugal, Romania, Russia, Ukraine, United Kingdom and Morocco).

— **Workshop on Neutron Holography** , Budapest, 10-12 November, 2005, organized by the Research Institute for Solid State Physics and Optics and Universität Wien, Chairman: Prof. L. Cser, Co-chairman, Prof. G. Krexner, 24 participants. The materials of the conference will be put on the web-page of the workshop: http://www.kfki.hu/~neuholo/workshop/.

— A meeting of the **COST Materials, Action P7: X-ray and neutron optics** has been held in Budapest, 13-15 October 2005, organized by the Neutron Spectroscopy department. The workgroup meeting offered the possibility for the 40 participants to present and discuss their recent results in the fields of theoretical calculations, surface preparation and tests, fabrication and testing of interferential mirrors, diffractive and refractive optics. Discussions about the future of this scientific network, installation of groups preparing the next application and administrative issues also constituted parts of the agenda.

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